

## Supplementary.Table.S1.

### Frequents Hitters

Diethylstilbestrol  
[CH3][C][C]([C]([C][CH3])[c]1[c][c][c]([O])[c][c]1)[c]2[c][c][c]([O])[c][c]2  
Triazolam  
[c]1([CH3])[n][n][c]2[C][N]=[C]([C]3[c][c][c][c]3Cl)[c]4[c][c](Cl)[c][c][c]4[n]12  
Apomorphine  
[CH3][N]1[C][C]2[C][C][C][C]-3[C]2[C]1[C][c]4[C][c][c]([O])[c]([O])[c]-34  
Idebenone  
[CH3][O][C]1[C]([O][CH3])[C](=O)[C]([C][C][C][C]([CH3])[C][C][C][C]([CH3])[C][O])[C]([CH3])[C]1=O  
Tocopherol  
[CH3][C]([CH3])[C][C][C][C]([CH3])[C][C][C][C]([CH3])[C][C][C][C]1([CH3])[C][C][c]2[c](-[CH3])[c]([O])[c](-[CH3])[c](-[CH3])[c]2[O]1  
Benserazide  
[N]([#1])([#1])[C]([C][O])[C](=O)[N][N][C][c]1[c][c][c]([O])[c]([O])[c]1[O]  
Clofazimine  
[CH3][C]([CH3])[N][C]1[C]=[c]2[c]([C]=[C]1[N][c]3[c][c][c](Cl)[c][c]3)[n][c]4[c][c][c][c]4[n]2[c]5[c][c][c]([CH3])[c][c]5  
Fenoterol  
[CH3][C]([C][c]1[c][c][c]([O])[c][c]1)[N][C][C]([O])[c]2[c][c]([O])[c][c]([O])[c]2  
Calciferol  
[CH3][C]([CH3])[C][C][C][C]([CH3])[C]1[C][C][C]2[C]1([CH3])[C][C][C]\[C]2=[C]/[C]=[C]3\[C][C]([O])[C][C][C]3[CH3]  
SF85190  
[#6][N]([C][C][C]#C[C]([CH3])([CH3])[CH3])[C][c]1[c][c][c][c]2[c][c][c][c]12  
Troglitazone  
[CH3]-[c]1[c]([CH3])[c]([CH3])[c]2[O][C]([CH3])([C][O][c]3[c][c][c]([C][C]4[S][C](=O)[N][C]4=O)[c][c]3)[C][C][c]2[c]1-[CH3]  
Dextrotiroxina  
[c]1[c]([c]([c][c][c]1[O])[c]1[c]([c][c]([c][c]1I)[C][C]([N]([#1])([#1]))C(O)=O)I)[O])I  
Methyldopamine  
[CH3][C]([#7H2])([C][c]1[c][c][c]([O])[c]([O])[c]1)[C]([O])=O  
Dopamine  
[#7][CH2][CH2][cX3]1[c][c]c([O])c([O])[c]1  
Dextrotiroxina-sodica  
[#7H2][C]([C][c]1[c][c](I)[c]([O][c]2[c][c](I)[c]([O])[c](I)[c]2)[c](I)[c]1)[C](O)=O

### Aggregators

3681\_1190  
C1c1ccc(COc2ccc(Br)cc2C=C2C(=O)NC(=O)NC2=O)cc1  
4854\_0030  
NC(=N)Nc1nc(cs1)c1ccc(O)c(O)c1  
1687\_0217  
C1c1cccc1c1nnc(NC(=O)c2cccs2)s1  
4896\_5245  
Brc1ccc2NC(=O)C(=Cc3cccc(OCC=C)c3)c2c1  
C155\_0360  
CC(C)CC(NC(=O)C1CCCC1)C(=O)Nc1cc(C)cc(C)c1  
4695\_1149  
O1c2ccccc2C(c2ccccc12)n1nnc2ccccc12  
2110\_0302  
CCOc1cc(C=C2SC(=S)N(NC(=O)c3ccccc3Cl)C2=O)ccc1O  
4112\_3656  
CN(C)c1ccc(Nc2nc(cs2)c2ccc(Cl)cc2)cc1  
C310\_1061  
COc1ccc(C=c2sc3ccc(cc3n(C)c2=O)C(=O)NCc2ccccc2)cc1  
C801\_0362  
Fc1ccc(cc1)n1ncc2c(=O)n(CC(=O)N3CCN(CC3)c3ccccc3)cnc12  
K781\_3644  
[O-]=N(=O)c1cc(ccc1N1CCN(CC1)c1cccn1)C(=O)NCc1cccs1  
0831\_0436  
O=C(Nc1nc(cs1)c1ccccc1)c1ccccc1  
Bisindolylmaleimide\_i  
[CH3][N]([CH3])[C][C][C][n]1[c][c]([C]2=[C]([C](=O)[N][C]2=O)[c]3[c][n]([CH3])[c]4[c][c][c][c][c]34)[c]5[c][c][c]15  
3643\_1650  
Cc1ccc(C=C(C#N)c2nc3ccccc3c(=O)[nH]2)cc1  
C224\_5057  
Cc1ccc(NC(=O)c2ccc(NC(=O)CCS(=O)(=O)c3cccs3)cc2)cc1  
8003\_5245  
Oc1cc(cc1)N1C(=O)c2cc3ccccc3c(c3ccccc3)c2C1=O  
3331\_3149  
C1c1ccc(cc1)N=C1C(=O)Nc2ccc(Br)cc12  
1687\_0292

BrC1ccc(cc1)c1nnc(NC(=O)c2cccs2)s1  
4264\_0007  
Oc1ccccc1C=NN=C1NC(=O)C(Cc2ccc(Cl)cc2)S1  
4476\_1849  
COC(=O)C1=C(C)NC(=C(C1c1oc(cc1)c1cc(Cl)ccc1Cl)C(=O)OC)C  
K788\_2054  
Coc1ccc(NC(=S)NCC2CCN(C2)c2ccc(OC)cc2)cc1  
8012\_8466  
CCOc1ccc2nc(SCC(=O)c3ccc(O)cc3)sc2c1  
5186\_0397  
Cc1cccn1Nc1nc(cs1)c1ccc(O)c(O)c1  
1814\_1801  
Oc1ccc(Br)cc1C=C1C(=O)Nc2ccccc12  
4554\_1325  
CCCCN(CC)S(=O)(=O)c1ccc(cc1)C(=O)Nc1ccc(cc1)c1[nH]c2ccccc2n1  
4476\_4106  
CCOC(=O)C1=C(C)NC(=C(C1c1cccc(Oc2ccccc2)c1)C(=O)OCC)C  
0800\_0109  
O=C(Nc1nc(cs1)c1ccc2ccccc2c1)c1ccccc1  
1814\_1806  
CCCCCc1cc(C=C2C(=O)Nc3ccccc23)c(O)cc1O  
5432\_0037  
Cn1cc(C(=O)NN=Cc2ccccc2O)c2ccccc12  
C336\_0015  
CCOc1ccc(NC(=O)CSc2nc3ccccc3c3=NC(C(=O)n23)c2ccccc2)cc1  
2159\_2474  
Coc1ccc(C=C2SC(=O)N(Cc3ccccc3)C2=O)cc1  
0657\_0230  
CCN(CC)c1ccc2cc(c(=O)oc2c1)c1csc(NN=Cc2ccccc2)n1  
3355\_0028  
Coc1ccc(cc1)C1CC(=NN1S(=O)(=O)c1ccccc1)c1ccccc1  
1331\_0061  
Cc1ccc(cc1)C(=O)NN1C(=S)SC(=Cc2ccccc2)C1=O  
5682\_0014  
Clc1ccc(CNC=C2C(=O)Nc3ccccc23)cc1  
5591\_2622  
CC(C)c1ccc(cc1)S(=O)(=O)N=C1C=C(Nc2ccc(O)cc2)C(=O)c2ccccc12  
Miconazole  
Cl[c]1[c][c][c]([c][O][c]([c][n]2[c][c][n][c]2)[c]3[c][c][c](Cl)[c][c]3Cl)[c](Cl)[c]1  
3253\_4022  
Oc1ccc(Br)cc1C=NNC(=O)c1cc([nH]n1)c1ccccc1  
3254\_3201  
[O-]=N(=O)c1cc(C=NNC(=O)c2cccs2)ccc1Cl  
1959\_0064  
C1C=CC2C1C(Nc1ccc3ccccc3c21)c1ccccc1  
2082\_0084  
Cc1ccc(cc1Cl)N1NC(=O)C(=Cc2ccccc2OCC=C)C1=O  
3254\_3286  
Oc1ccc(C=NNC(=O)c2cc([nH]n2)c2ccc3ccccc3c2)cc1O  
3209\_0258  
Cc1c(Cl)c(nn1CC(=O)Nc1ccccc(Cl)c1)C(F)(F)F  
0844\_0233  
Oc1ccccc1C=NNC(=O)c1ccccc1N(=O)=[O-]  
8006\_5314  
Oc1ccc(Br)cc1C=Nc1ccccc2c(=O)[nH][nH]c(=O)c12  
8005\_8816  
Oc1c(Cl)cc(Cl)cc1C=NNc1nc(cs1)c1ccccc1  
5311\_0132  
CCOc1ccc(C=C2C(=O)Nc3ccccc23)cc1  
8003\_9574  
Oc1c(I)cc(I)cc1C=Nc1ccc(cc1)N(=O)=[O-]  
2783\_5196  
[O-]=N(=O)c1cc(ccc1Cl)C(=O)Nc1ccc(NC(=O)c2ccccc2)cc1  
8003\_3961  
Nc1ccccc(Oc2ccc3C(=O)N(C(=O)c3c2)c2ccccc2)c1  
Rottlerin  
[CH3][C](=O)[c]1[c]([O])[c]([CH3])[c]([O])[c]([C][c]2[c]([O])[c]([C](=O)/[C]=[C]/[c]3[c][c][c][c]3)[c]4[O]  
[C]([CH3])([CH3])[C]=[C][c]4[c]2[O])[c]1[O]  
8013\_1565  
O=C(Nc1ccccc1)c1ccc(c1)S(=O)(=O)NCCC12CC3CC(CC(C3)C1)C2  
2276\_0149  
CCOC(=O)c1sc(NC(=O)Coc2ccc(CC)cc2)nc1C  
3289\_1461  
OC(=O)c1ccc(Oc2ccc3C(=O)N(C(=O)c3c2)c2ccc(Oc3ccccc3)cc2)cc1  
C280\_0321  
CC1Cc2c(S1)c(=O)n(Cc1ccccc1)c(n2)SCC(=O)Nc1ccccc1  
1502\_1187  
Oc1cc2ccccc2cc1C(=O)NN=Cc1oc(cc1)c1ccc(Cl)cc1  
2681\_3685

[O-]=N(=O)c1cccc(C=C(NC(=O)c2cccs2)C(=O)Nc2ccccc2Br)c1  
4296\_0709  
CC1=C(C(C(=C(N1)SCC(=O)Nc1ccc(Cl)c(Cl)c1)C#N)c1occc1)C(=O)N  
3738\_4387  
O=C(Nc1ccc(NC(=O)c2cccs2)cc1)c1oc2ccccc2c1  
2\_05  
[CH3][C]([CH3])[C][C]([O][c]1[c][c][c]([O][C](=O)[c]2[c][c]([n][c]([c]2)[c]3[c][c][c][c](Cl)[c][c]3)[c]4[c][c][c]  
)(Cl)[c][c]4)[c][c]1)[C]([O])=O  
2\_04  
[CH3][C][C][C][c]1[c][c][c]([c][c]1)[c]2[c][c]([c][c]([n]2)[c]3[c][c][c](Cl)[c][c]3)[C]([O])=O  
2\_07  
[C][O][c]1[c][c][c]2[C]3[C][C][C]4([C])[C]([C][C][C]4[C]3[C][C][c]2[c]1)[N][C][C][N][c]5[c][c][c]([c][n]5)[N+]  
](=O)[O-]  
2\_06  
[CH3][c]1[c][c][c]([c][c]1)[c]2[c][c]([c][c]([n]2)[c]3[c][c][c]4[c][c][c][c]4[c]3)[C]([O])=O  
2\_01  
[O][C](=O)[c]1[c][c]([n][c]([c]1)[c]2[c][c][c]([S][c]3[c][c][c](Cl)[c][c]3)[c][c]2)[c]4[c][c][c](Cl)[c][c]4  
4356\_1378  
Clc1ccc(NC2=NC(=O)C(=C3C(=O)Nc4ccccc34)S2)cc1  
2\_03  
[O][C](=O)[c]1[c][c]([n][c]([c]1)[c]2[c][c][c]([c][c]2)[c]3[c][c][c][c]3)[c]4[c][c][c](Cl)[c][c]4  
2\_02  
[CH3][C]([CH3])([CH3])[c]1[c][c][c]([c][c]1)[c]2[c][c]([c][c]([n]2)[c]3[c][c][c](Cl)[c](Cl)[c]3)[C]([O])=O  
3229\_1438  
Clc1ccc(Sc2ccccc2C=C2SC(=O)NC2=O)cc1  
3254\_3578  
Oc1ccc(C=NNC(=O)c2cc([nH]n2)c2ccc(OCc3ccccc3)cc2)cc1  
2738\_0167  
CCOc1ccc(cc1)N=C1SC(CC(=O)N1Cc1ccccc1)C(=O)Nc1ccccc1OC  
D030\_0006  
O=S(=O)(NCC(Nc1ccccc1)c1ccccc1)c1ccccc1  
2\_09  
[CH3][O][C]1[C][C][C]2([CH3])[C]([C][C][C]3[C]4[C][C][C]([N][C][C][N]([#1]))[C]4([CH3])[C][C]([O])[C]23)[C]1  
2\_08  
[CH3][O][c]1[c][c][c]2[C]3[C][C][C]4([CH3])[C]([C][C][C]4[C]3[C][C][c]2[c]1)[N][C][C][C][c]5[c][c][c][c][c]5  
K939\_0042  
Cc1ccc2NC(=O)C(=Cc3ccc(cc3)C(C)(C)C)c2c1  
3254\_3219  
[O-]=N(=O)c1ccc(Cl)c(C=NNC(=O)c2cccs2)c1  
4358\_4590  
COc1ccc(Nc2nc(nc3ccccc23)c2ccc(cc2)N(=O)=[O-])cc1  
C549\_0174  
CSc1cccc(NC(=O)c2nnn(Cc3ccc(F)cc3)c2N)c1  
3736\_0402  
COc1ccc2[nH]c(SCc3cccc(I)c3)nc2c1  
3254\_4008  
Cc1ccc(s1)c1cc([nH]n1)C(=O)NN=Cc1ccccc1  
K939\_0049  
Cc1ccc2NC(=O)C(=Cc3ccc(Br)cc3)c2c1  
4076\_0222  
CC(C)Oc1ccc(cc1)c1cc([nH]n1)C(=O)NN=Cc1ccccc1O  
2023\_0191  
[O-]=N(=O)c1ccc(Cl)cc1NCCOc1ccccc1  
4191\_2977  
COc1ccccc1NC(=O)CN(CCc1ccccc1)S(=O)(=O)c1ccccc1  
8007\_0609  
COc1ccc2oc(=O)c(cc2c1)c1csc(Nc2cccc3ccccc23)n1  
4896\_5304  
CSc1ccc(C=C2C(=O)Nc3ccc(Br)cc23)cc1  
0393\_0188  
Oc1ccccc1C=Nn1c2ccccc2c2ccccc12  
8005\_6509  
Brc1cccc(c1)C(=O)Oc1ccc(C=NNC(=O)c2ccnc2)cc1  
C131\_0032  
Brc1ccc2NC(=O)C(=Cc3ccccc3)c2c1  
3720\_3614  
Cn1cc(C=C2C(=O)NC(=S)NC2=O)c2ccccc12  
K284\_0591  
COc1ccccc1Cn1c(nc2ccccc2c1=O)SCC#N  
4896\_5188  
OC(=O)COc1ccc(Br)cc1C=C1C(=O)Nc2ccc(Br)cc12  
4554\_6348  
CCOc1ccc(cc1)C1CC(=O)NC(=C1C#N)SCC(=O)Nc1ccccc1C)c1  
4449\_1925  
Clc1ccc(Sc2oc(C=C3NC(=O)NC3=O)cc2Br)cc1  
8006\_5812  
Clc1ccc(CSc2nnnn2c2ccccc2)cc1  
2180\_0282  
Oc1ccccc1C=NNC(=O)COc1ccc(Cl)cc1

3388\_0871  
O=C(Nc1nnc(CSCc2ccccc2)s1)c1cccs1  
5895\_0010  
Oc1ccc(C=C2C(=O)ON=C2c2ccc(Cl)cc2)cc1  
5275\_0031  
CCCC(=O)NC(c1ccccc1)c1cc(Cl)c2ccnc2c10  
8005\_8620  
Oc1ccc2ccccc2c1C=NNc1nc(cs1)c1ccccc1  
0896\_4285  
Oc1ccccc1C=NNC(=O)C(=O)NN=Cc1ccccc10  
3254\_0603  
Oc1ccc(C=NNC(=O)CSc2nnc(c3ccc(Cl)cc3)n2c2ccccc2)cc10  
3330\_3565  
Clc1ccc(cc1)C(=O)Nc1c2CScc2nn1c1ccccc1  
5298\_5553  
CC1(C)CC(=O)c2sc(NC(=O)C=Cc3ccccc3Cl)nc2C1  
3332\_1138  
COC(=O)CN1C(Nc2ccc(Br)cc2C1c1ccccc1)c1ccc(O)cc1  
C444\_2160  
CCC(=O)N1CCCc2cc(ccc12)S(=O)(=O)N1CCC(=CC1)c1ccccc1  
Benzyl\_benzoate  
O=C([O][C][C]1[C][C][C][C][C]1)[C]2[C][C][C][C][C]2  
8003\_2415  
Cc1ccc(OCc2ccc(cc2)C(=O)NN=Cc2ccccc2O)cc1  
Indirubin  
O=C1[N][C]2[C][C][C][C][C]2\ [C]1=[C]3\ [N][C]4[C][C][C][C][C]4[C]3=O  
0389\_1021  
COC1ccc(cc1)C(=O)Nc1nc(cs1)c1ccccc1OC  
6049\_2574  
CCOc1ccccc1c1cc(C(=O)Nc2ccc(cc2)S(=O)(=O)N)c2ccccc2n1  
3254\_3800  
Oc1ccccc1C=NNC(=O)c1cc([nH]n1)c1ccc(Cl)cc1Cl  
1900\_2706  
COC1cc(OC)cc(c1)C(=O)N1c2ccccc2Sc2ccccc12  
8008\_3055  
C(OC1ccc(C=NNc2nnnn2c2ccccc3ccccc23)cc1)c1ccccc1  
5186\_0398  
NS(=O)(=O)c1ccc(Nc2nc(cs2)c2ccc(O)c(O)c2)cc1  
U0126  
[N]([#1])/[C](=[C]/[C]#[N])[C](=[C]/[N]([#1]))[S][c]1[c][c][c][c][c]1[N]([#1])[C]#[N])/[S][c]2[c][c][c][c][c]  
[c]2[N]([#1])  
3253\_4328  
CC(=NNC(=O)c1[nH]nc2c1CCc1ccccc21)c1ccccc2ccccc12  
1906\_0077  
Cc1ccccc1Nc1nc(cs1)c1ccc(Cl)cc1  
1\_13\_2  
[#7]-[c]1[c]([c][c]([c]2[c][c][c][c][c]12)S([#8-])(=O)=O)N=N[c]3[c][c][c]([c]1[c]3)-  
[c]4[c][c][c]([c]([c]4)N=N[c]5[c][c]([c]6[c][c][c][c]6[c]5-[#7])S([#8-])(=O)=O  
0422\_0061  
Cc1ccc(cc1)S(=O)(=O)Nc1ccc(Br)c2ccnc12  
K007\_0498  
NS(=O)(=O)c1ccc(NN=C(c2ccccc2)c2ccc(Br)cc2)cc1  
1185\_0334  
COC1ccc(C=NNc2nc(cs2)c2ccc(Cl)cc2)cc1  
4371\_6384  
Clc1ccc(CN2C(=O)NC(=Cc3ccc(OCc4ccccc4)cc3)C2=O)cc1  
0485\_0277  
Ic1ccc(cc1)c1csc(NC(=O)C=Cc2ccccc2)n1  
2\_18\_3  
[O][C](=O)[C][O][c]1[c][c][c]([c][c]1)N=N[c]2[c][c][c]3[c][c](Br)[c][c][c]3[c]2[O]  
C127\_0095  
CCc1ccc2nc(sc2c1)N1CCC(CC1)C(=O)NCCC(C)C  
1683\_4862  
CCOc1ccccc1NC(=O)COc1ccc(cc1)C(C)C  
C131\_0029  
Cc1ccccc1C=C1C(=O)Nc2ccc(Br)cc12  
8012\_3364  
COC1cc2c(oc3ccccc23)cc1NC(=O)COc1ccc2ccccc2c1  
2124\_0315  
[O-]=N(=O)c1ccccc(C=CC2=NC(=CNC3ccc4ccccc4c3)C(=O)O2)c1  
5186\_0241  
COC1ccc(cc1C)c1csc(Nc2ccccc(C)n2)n1  
3202\_0050  
CN(C)c1ccc(Sc2nnc(NC(=O)c3ccc(Cl)cc3)s2)cc1  
4489\_8151  
[O-]=N(=O)c1ccccc(COC2ccc(C=C3C(=O)NC(=O)NC3=O)cc2Br)c1  
3272\_1158  
Cc1ccccc1NC(=O)c2ccc(cc2)N(Cc2ccccc2)S(=O)(=O)C)c1  
0547\_0134

BrC1ccc(cc1)c1csc(NC(=O)c2cccs2)n1  
K252c  
O=C1[N][C][C]2[C]1[C]3[C]4[C][C][C][C]4[N][C]3[C]5[N][C]6[C][C][C][C]6[C]25  
K801\_0927  
CCOC(=O)N1CCc2c(Cl)sc(NCc1cccs1)c2C(=O)Nc1ccccc1OCC  
C434\_0009  
FC(F)(F)c1cccc(NC(=O)Cn2ncc3c(=O)oc4ccccc4c23)c1  
6228\_1083  
Nn1c(=O)c2ccccc2nc1c1cccc(COc2ccccc2Br)c1  
5149\_0176  
CCN1C(=C(OC(=O)c2ccccc2)c2ccccc2S1(=O)=O)C(=O)c1ccccc1  
C638\_0047  
Clc1ccc(cc1)C(=O)Nc1cccc(c1)c1cn2cccn2n1  
3261\_0589  
[O-]=N(=O)c1ccc(cc1)C(=O)Nc1ccccc1C(=O)Nc1ccccc1  
1936\_2266  
CN(C)c1ccc(C=C(NC(=O)c2ccccc2)C(=O)NN=Cc2ccccc2O)cc1  
Delavirdine  
[CH3][C]([CH3])[N][c]1[c][c][n][c]([c]1)[N]2[C][C][N]([C][C]2)[C](=O)[C]3[C][c]4[c][c]([N][S](=O)(=O)[CH3])[c]  
][c][c]4[N]3  
4137\_1362  
Clc1ccc(cc1)cloc(cc1)C(=O)Nc1ccc(NC(=O)c2occc2)cc1  
8007\_4133  
Oc1ccc(Cl)cc1C=NNC(=O)C(=Cc1ccccc1)NC(=O)c1ccccc1  
1699\_1961  
Oc1ccc(Br)cc1C=NNC(=O)c1ccccc1)c1  
C453\_0208  
COc1cccc(c1)c1nn(C)c2sc(cc12)C(=O)NCc1ccc(C)cc1  
8004\_2736  
Oc1ccc(Br)cc1C=Nc1cccc2ccccc12  
3254\_3297  
[O-]=N(=O)c1ccc(Cl)c(C=NNC(=O)c2cc([nH]n2)c2ccc3ccccc3c2)c1  
2293\_4303  
Cc1ccc(cc1)c1csc(Nc2ccccc2Cl)n1  
8001\_9289  
CN(C)c1ccc(C=C(NC(=O)c2ccccc2Cl)C(=O)NN=Cc2ccccc2O)cc1  
K786\_3182  
O=C(CCc1cn(Cc2ccccc2)c2ccccc12)NCc1ccccc1  
C085\_1642  
COc1ccccc1N1CCN(CC1)S(=O)(=O)c1ccc(Br)s1  
4554\_6401  
Clc1ccc(cc1)C1C(=C(NC2=C1C(=O)CCC2)SCC(=O)Nc1ccccc1)C#N  
K781\_2996  
CC1CCCN1C(=O)c1ccc(Sc2ccc(F)cc2)c(c1)N(=O)=[O-]  
1\_08  
[#8-][C](=O)[c]1[c][c][c][c][c]1\C[C]([C]2[C][c](I)[c](-[#8-])[c](I)[C]2)=[C]3\C[C]=[C](I)[C](=O)[C](I)=[C]3  
1\_09  
[O-][c]1[c](I)[c][c]2[c]([O][c]3[c](I)[c]([O-]  
])[c](I)[c][c]3[C]2[c]5[c]([C](=O)O[#1])[c](Cl)[c](Cl)[c](Cl)[c]5Cl)[c]1I  
8002\_5376  
[O-]=N(=O)c1cc(cc(c1)N(=O)=[O-])C(=O)Oc1ccc(cc1)C(=O)OCc1ccccc1  
2262\_4150  
Oc1ccc(Br)cc1C=NNC(=O)c1cc(cc(c1)N(=O)=[O-])N(=O)=[O-]  
K832\_1618  
[O-]=N(=O)c1cccc(c1)C1C=C(Nc2nnnn12)c1ccc(Cl)cc1  
4896\_5243  
CCOc1ccc(Br)c(C=C2C(=O)Nc3ccc(Br)cc23)c1  
8008\_7159  
COc1cccc(C=C2SC(=Nc3ccc(C)cc3)NC2=O)c1  
1\_01  
[Cl][c]1[c][c][c]2[s][c]([S][c]3[n][n][c]([N][C](=O)[c]4[c][c][c]([Cl])[c]([Cl])[c]4)[s]3)[n][c]2[c]1  
1\_02  
[O][c]1[c][c][c]([N]=[N][c]2[c][c][c](Br)[c][c]2)[c]1  
1\_03  
[O]=[C]1[O]/[C](=[C][N][c]2[c][c][c]([O][c]3[c][c][c][c]3)[c][c]2)/[c]4[c][c][c][c]14  
1\_04  
[O][c]1[c][c][c][c]1[C]=N[N][C](=O)[C](=O)[N]N=[C][c]2[c][c][c][c]2[O]  
1\_05  
[CH3][c]1[c][c](Cl)[c][c]2[S]/[C](=[C]3/[S][c]4[c][c](Cl)[c][c]([CH3])[c]4[C]3=O)/[C](=O)[c]21  
1\_06  
[O][c]1[c][c][c]2[c][c][c][c]2[c]1N=N[c]3[c](O)[c][c]([c]4[c][c][c][c]34)S([#8-])(=O)=O  
1\_07  
[O][c]1[c][c]([c]2[c][c][c][c]2[c]1N=N[c]3[c][c][c]4[c][c][c][c]4[c]3[O])S([#8-])(=O)=O  
4896\_1256  
CC(C)(C)c1cc(C=C2C(=O)NC(=O)NC2=O)cc(c1O)C(C)(C)C  
3253\_2326  
Oc1ccc2ccccc2c1C=NNC(=O)c1cc([nH]n1)c1ccc2ccccc2c1  
C094\_0212  
COc1ccc(cc1)C(NC(=O)Cc1cccs1)C(=O)Nc1ccc2OCCOc2c1

C226\_4061  
COc1ccc2c(Cc3c2onc3C(=O)Nc2cccc(O)c2)c1  
Econazole  
Cl[c]1[c][c][c]([c][O][C]([c][n]2[c][c][n][c]2)[c]3[c][c][c](Cl)[c][c]3Cl)[c][c]1  
4321\_1036  
O=C(Nc1ccc(cc1)c1nc2cccc2s1)c1cccc1  
8003\_8143  
[O-]=N(=O)c1ccc(NN=Cc2ccc3NCCc3c2)c(c1)N(=O)=[O-]  
K783\_0188  
COC(=O)c1ccc(N2CCc3cccc23)c(c1)N(=O)=[O-]  
4896\_5349  
COc1cc(C=C2C(=O)Nc3ccc(Br)cc23)cc(Cl)c1  
C064\_0401  
[O-]=N(=O)c1ccc(CSc2cn(CCNC(=O)c3cccs3)c3cccc23)cc1  
C137\_2180  
Brc1ccc(NS(=O)(=O)c2cc(Br)cc3CCN(C(=O)C4CC4)c23)cc1  
1000\_0257  
[O-]=N(=O)c1cccc(c1)C(=O)Nc1nc(cs1)c1ccc(Cl)c(Cl)c1  
K284\_1926  
Cc1ccc(NC(=O)CSc2nc3cccc3c(=O)n2Cc2occc2)cc1  
8008\_8367  
CCC1SC(=NN=C(C)c2ccc(Br)cc2)NC1=O  
1130\_0084  
O=C(CCc1cccc1)Nc1sc2CCCCc2c1C#N  
3772\_6188  
Nc1c(sc2nc3CCCCc3cc12)C(=O)Nc1cccc1  
3453\_0991  
Cc1cccc(N2C(=O)C(=C(Nc3cccc3)C2=O)Cl)c1C  
K786\_5352  
CCCCSCCCNC(=O)Nc1ccc(Cl)c(Cl)c1  
3341\_1057  
CC(C)Oc1ccc(cc1)C(=O)Nc1cccc(c1)c1[nH]c2cccc2n1  
3253\_0411  
Brc1ccc(C=NNC(=O)c2cccs2)cc1  
C285\_0027  
Brc1ccc(NC=C2C(=O)Nc3cccc23)cc1  
5871\_1853  
Cc1ccc(Oc2ccc3C(=O)N(C(=O)c3c2)c2ccc(cc2)C(=O)O)cc1  
8010\_0526  
Cc1ccc(OCCSc2nc(=O)c3cccc3[nH]2)cc1  
5350\_0194  
COc1ccc(cc1)c1ccc2c(N)c(sc2n1)C(=O)Nc1cccc1C  
1426\_2791  
Cc1ccc(NC(=O)c2cc3c(C)nn(c4cccc4)c3s2)cc1  
2154\_0429  
[O-]=N(=O)c1ccc(Cl)c(c1)C(=O)Nc1cccc(NC(=O)c2cccc2Cl)c1  
8005\_9141  
CCOC(=O)Cl=C(C)N(C(=O)Cl=Cc1ccc(OC)cc1)c1cccc1  
1761\_2016  
COc1ccc(cc1)C(=O)NN=Cc1cc(Cl)ccc1O  
5948\_4338  
COc1ccc(Br)cc1C1C(=C(N)Oc2cc3OCOc3cc12)C#N  
1693\_0015  
COc1cc(C=NNC(=O)Cn2c3cccc3c(=O)c3cccc23)ccc1O  
3253\_0416  
Oc1c(Br)cc(Br)cc1C=NNC(=O)c1cccs1  
4077\_0257  
Brc1ccc2OC3(CCCC3)N3N=C(CC3c2c1)c1cccs1  
1\_12  
[O][c]1[c][c][c]([c][c]1[O])[c]2[c][s][c]([N][c]3[c][c][c](F)[c][c]3F)[n]2  
1\_11  
[O][N+](=O)[c]1[c][c][c]([N][N]2[C](=O)[C]3[C]([C]2=O)[C]4(Cl)[C](=[C](Cl)[C]3(Cl)[C]4(Cl)Cl)Cl)[c]([c]1)[N+]  
(=O)[O-]  
1\_10  
[CH3][C]([CH3])[c]1[c][c][c]/[C]=[C]2/[C](=O)[N][c]3[c][c][c][c][c]23)[c][c]1  
1184\_1702  
[O-]=N(=O)c1ccc(NN=c2c(=O)c3cccc3c2=O)c(c1)N(=O)=[O-]  
4151\_0542  
Cc1ccc(NC(=O)C2CC(=O)N=C(Nc3ccc(C)cc3)S2)cc1  
3572\_4569  
O=C1N(Cc2cccc2)c2c([nH]nc12)c1cccc1)c1cccc1  
3235\_0039  
Brc1ccc2NC(=O)C(=Nc3ccc4cccc4c3)c2c1  
8002\_2154  
[O-]=N(=O)c1cccc(c1)C(=O)Oc1ccc(C=NNC(=O)c2cccc(Br)c2)cc1  
2043\_6447  
CCOc1cccc1C(=O)Nc1cc(Cl)ccc1Cl  
C094\_0141  
CCN(C(=O)Nc1ccc(OC)cc1)c1cc2OCOc2cc1N(=O)=[O-]c1cccc(C)c1

2181\_1127  
BrC(=Cc1cccc1)C=NNC(=O)CNc1cccc2cccc12  
0663\_0335  
Cc1cccc(NC(=O)c2ccc(cc2)S(=O)(=O)N2CCCC2)c1  
4456\_0561  
O=C1c2cccc2C(=O)c2c1cccc2S(=O)(=O)Nc1cccc1  
0945\_0278  
Cc1cccc(Nc2nc(cs2)c2cccc2)c1  
C131\_0049  
Clc1ccc(C=C2C(=O)Nc3ccc(Cl)cc23)cc1  
Indigo  
O=[C]1[c]2[c][c][c][c][c]2[N]\[C]1=[C]3\[N][c]4[c][c][c][c]4[C]3=O  
4157\_1124  
COc1ccc(C=C2Cc3cc(OC)ccc3C2=O)cc1  
0384\_0038  
Nc1ccc(cc1)C1(c2ccc(N)cc2)c2cccc2c2cccc12  
1252\_1580  
Oc1ccc2cccc2c1C=Nc1ccc(C=C)cc1  
5223\_6433  
CCOc1cc(O)c(cc1CC)c1[nH]ncc1c1cccc1  
C730\_0394  
Cc1ccc(NC(=O)C(=O)c2c(C)[nH]c3cccc23)cc1C  
5750\_1180  
CCOc1ccc2nc(NC(=O)COc3cccc3)sc2c1  
1523\_5774  
Oc1ccc(Cl)cc1C=NNC(=O)c1cccs1  
3002\_1335  
CC1CCN(CC1)c1nc(nc2cccc12)c1cccc1  
0584\_0340  
O=C(OC(=O)c1cccc1)C(c1cccc1)c1cccc1  
3993\_4237  
CN(C)c1ccc(NC(=O)c2oc3cccc3c2)cc1  
3330\_4053  
CCOc1ccc2c(cc(=O)oc2c1)c1cccc1  
4476\_0252  
CC1=C(C(C(=C(N1)C(=O)OCC=C)c1cccc(c1)N(=O)=[O-])C(=O)OCC=C  
0350\_0137  
Oc1cccc1C=NN=CC=Cc1cccc1  
8009\_3091  
CCSc1nc2ccc(NC(=O)CSc3nc4ccc(N)cc4s3)cc2s1  
3226\_2061  
Cc1ccc(C)c1OCC(=O)Nc1ccc(cc1)c1[nH]c2cccc2n1  
2357\_3050  
O=C(NN=Cc1c[nH]c2cccc12)c1cc([nH]n1)c1ccc(OCc2cccc2)cc1  
0054\_0133  
CCCC1CCC(CC1)c1ccc(cc1)C(=NO)N  
2291\_3304  
CCCOc1ccc(cc1)C(=O)C(=c1[nH]c2cccc2[nH]1)C#N  
K072\_0220  
Cc1ccsc1C=NNc1nc2cccc2s1  
K284\_5355  
CC1CN(CCN1c1cccc(C)c1)C(=O)CCn1c(=S)[nH]c2cc3OCOc3cc2c1=O  
2108\_1341  
Oc1ccc(Br)cc1C=NNC(=O)c1ccc(Cl)cc1Cl  
2\_20  
[C]1[C][N][C][C]([C]1)[C]=[C]2[C]3[C][C][C][C][C]3[C]4[C][C][C][C][C]24  
1588\_0383  
OC(=O)c1ccc(cc1)c1oc(C=C2SC(=O)N(C2=O)c2cccc2)cc1  
C656\_0069  
Cc1ccc(Cn2nnc3c(=O)n(Cc4cc(C)ccc4C)cnc23)cc1  
1488\_0481  
Clc1ccc(cc1)c1csc(NC(=O)c2cccc(Cl)c2)n1  
3339\_4762  
Fc1ccc(cc1)C(=O)Nc1nc2c(cc3CCc4cccc2c34)s1  
8002\_2326  
Clc1ccc(COc2ccc(C=NNC(=O)C(=O)Nc3cccc(Br)c3)cc2)cc1  
C175\_0112  
CCOC(=O)c1[nH]c2cccc2c1NC(=O)c1ccc2cccc2c1  
3003\_0752  
CCc1ccc(cc1)S(=O)(=O)N1CCN(CC1)c1cccc1  
1761\_1089  
CCC(=NNC(=O)CCC(=O)Nc1ccc(I)cc1)Cc1cccc1  
0800\_0121  
O=C(Nc1nc(cs1)c1ccc2cccc2c1)c1cccs1  
C145\_0016  
Cn1c(nc2c([nH]c3cccc23)c1=O)SCC(=O)Nc1cccc1  
1889\_2996  
CCOC(=O)Cl=C(C)NC(=C(Cl)c1oc(cc1)c1ccc(Cl)cc1)C(=O)OCC)C  
C270\_0212

Cc1ccc(Cl)cc1N1CCN(CCNC(=O)Nc2ccccc2)CC1  
3771\_8282  
BrC1CCCC(c1)C(=O)NC(=Cc1occcc1)C(=O)Nc1ccccc1  
K229\_0982  
COc1cccc(C=CC(=O)c2cc3ccccc3oc2=O)c1  
2237\_0104  
CC(C)(C)c1ccc(cc1)c1nnc(NC(=O)c2cccs2)s1  
0800\_0128  
[O-]=N(=O)c1cccc1C(=O)Nc1nc(cs1)c1ccc2ccccc2c1  
8008\_6103  
Oc1ccc(C=NNC(=O)C(=O)Nc2cc(Cl)ccc2Cl)c(O)c1  
8008\_6105  
Oc1ccc2ccccc2c1C=NNC(=O)C(=O)Nc1cc(Cl)ccc1Cl  
0325\_0403  
Oc1ccc(N=Nc2ccc(cc2)N(=O)=[O-])c2ccccc12  
0080\_0066  
CC1=C(COC2c3oc(=O)ccc3cc3ccoc23)CC(C)(C)CC1  
2712\_3260  
CCOC(=O)c1c(C)c(C)sc1NC(=O)Cc1cccc2ccccc12  
8008\_5856  
CC(=O)N=C1NC(=O)C(=Cc2oc(cc2)c2cccc(Cl)c2)S1  
Sulconazole  
Cl[c]1[c][c][c]([c][s][c]([c][n]2[c][c][n][c]2)[c]3[c][c][c](Cl)[c][c]3Cl)[c][c]1  
8007\_8341  
Oc1c(C=NNC(=O)c2cccc(Cl)c2)ccc2ccccc12  
0590\_0525  
[O-]=N(=O)c1ccc2[nH]c(=O)c(c3ccccc3)c2c1)C(=O)C=Cc1ccccc1  
Quercetin  
[O][c]1[c][c]([c]([O])[c]2[c](=O)[c]([O])[c]([O][c]2[c]1)[c]3[c][c][c]([O])[c]([O])[c]3  
2357\_3049  
[O-]=N(=O)c1ccc(C=NNC(=O)c2cc([nH]n2)c2ccc(OCc3ccccc3)cc2)cc1  
C301\_0220  
COc1cc(Cl)c(C)cc1Nc1c(nn(c2cccc(C)c2)[n+]1[O-])N(=O)=[O-]  
K783\_3251  
CCOC(=O)CCN(Cc1ccc(F)cc1)S(=O)(=O)c1ccc(Cl)cc1  
K939\_0013  
CC(C)c1ccc(C=C2C(=O)Nc3ccccc23)cc1  
K091\_1157  
[O-]=N(=O)c1cc(NC=C2N=C(OC2=O)c2ccc(Br)cc2)ccc1Cl  
3253\_2866  
Clc1ccc(cc1)c1cc([nH]n1)C(=O)NN=Cc1c[nH]c2ccccc12  
8001\_2346  
Clc1ccc(COc2ccc(cc2)C(=O)NN=Cc2c[nH]c3ccccc23)cc1  
2\_19  
[#6][c][c][c][c][c][c]([O][c]1[c][c][c]([c][c]1)S(=O)(=O)[c]2[c][c][c]([O][c]3[c][c][c][c]3)[c][c]2)[c]  
([O])=O  
Clotrimazole  
Cl[c]1[c][c][c][c][c]1[C]([c]2[c][c][c][c]2)([c]3[c][c][c][c]3)[n]4[c][c][n][c]4  
4111\_0016  
N#Cc1ccc(cc1)C1Oc2ccccc2C2CC(=NN12)c1ccccc1  
3253\_0361  
O=C(NN=Cc1cccc(OCc2ccccc2)c1)c1cccs1  
2\_12  
[CH3][N]([CH3])[c]1[c][c][c]/[C]=[C]2/[C](=O)[N][c]3[c][c][c][c][c]23)[c][c]1  
2\_13  
[O][c]1[c]([c]([c]2/[C](=O)[N][c]3[c][c][c][c]23)[c][c]4CCCCc14  
2\_10  
O=[C]/1[N][c]2[c][c][c][c]2[C]1=[C][c]3[c][c][c]([s]3)[c]4[c][c][c][s]4  
2\_11  
[CH3][C]([CH3])([CH3])[c]1[c][c]([c]([c]2/[C](=O)[N][c]3[n][c][c][c][c]23)[c][c]([c]10)[C]([CH3])([CH3])[CH3  
]  
2\_16  
[C]([#1])([#1])([#1])[c]1[c][c](Cl)[c][c]2[S][C]([C](=O)[c]12)=[C]3[S][c]4[c][c](Cl)[c][c]([C]([#1])([#1])([#  
1]))[c]4[C]3=O  
2\_17  
[O][c]1[c](N=N[c]2[c][c][c](Br)[c][c]2S([#8-])(=O)=O)[c]([c][c]3[c][c]([c](N=N[c]4[c][c][c](Br)[c][c]4S([#8-  
]))(=O)=O)[c](O)[c]13)S([#8-])(=O)=O)S([#8-])(=O)=O  
2\_14  
Cl[c]1[c][c][c]2[s][c]([s][c]3[n][n][c]([N][C](=O)[c]4[c][c][c][s]4)[s]3)[n][c]2[c]1  
2\_15  
[O][c]1[c][c][c]([N]=[N][c]2[c][c][c][c](Br)[c]2)[c][c]1  
1187\_1046  
CN(C)c1oc(nc1S(=O)(=O)c1ccc(C)cc1)c1ccccc1  
C331\_0385  
COc1ccc(cc1)c1[nH]c(SCC(=O)NCc2occc2)c(n1)c1ccccc1  
8011\_8270  
O=C1OC2(CCCC2)OC(=O)C1=Cc1ccc(OCc2ccccc2)cc1  
C224\_2833  
CCc1ccc(NC(=O)CNS(=O)(=O)c2ccc(Br)s2)cc1

2513\_0502  
 Cc1ccc(cc1)S(=O)(=O)Nc1cccc1C(=O)Nc1nc(cs1)c1ccc(F)cc1  
 K220\_48090  
 CCOC1cccc2cc(C(=O)Nc3cccc(c3)C(F)(F)F)c(=Nc3ccc(cc3)C(=O)O)oc12  
 C189\_0341  
 Cc1cccc1Cn1cc(c2cccc12)S(=O)(=O)CC(=O)NC1CCCC1  
 0945\_0604  
 BrC1ccc(cc1)c1csc(NN=Cc2ccccc2)n1  
 4469\_0604  
 Clc1ccc(cc1)c1csc(NCc2ccccc2)n1  
 0945\_0607  
 CN(C)c1ccc(C=NNc2nc(cs2)c2ccc(Br)cc2)cc1  
 Ro318220  
 [CH3][n]1[c][c]([C]2=[C]([C](=O)[N][C]2=O)[c]3[c][n]([C][C][C][S][C]([N]([#1]))=[N])[c]4[c][c][c][c][c]34)[c]  
 5[c][c][c][c][c]15  
 3253\_1842  
 COc1cccc1C=NNC(=O)c1cc([nH]n1)c1ccccc1  
 3391\_6686  
 CCOC1ccc(Nc2nc(Cl)nc(Nc3ccc(OC)c(OC)c3)n2)cc1  
 4171\_0235  
 CC1=NOC(=O)C1=Cc1ccc(OCc2ccc(Cl)cc2)cc1  
 4514\_0614  
 CCN1C(=O)CC(SC1=Nc1ccc(F)cc1)C(=O)Nc1ccc(Br)cc1  
 K292\_0969  
 COc1cccc(NC(=O)CSc2nc3ccsc3c(=O)n2C2CCCC2)c1  
 2154\_0028  
 FC(F)(F)c1cccc(NC(=O)c2cc(Br)ccc2Cl)c1  
 4476\_0270  
 CC1=C(C(C(=C(N1)C(=O)OCC=C)c1cccc(Cl)c1)C(=O)OCC=C  
 6143\_0170  
 Cc1ccc(NC(=O)C2Cc3ccccc3CN2S(=O)(=O)c2ccc(C)cc2)cc1  
 Nicardipine  
 [CH3][O][C](=O)[C]1=[C]([CH3])[N][C]([CH3])=[C]([C]1[c]2[c][c][c][c]([C]2)[N+])([O-]  
 )=O)[C](=O)[O][C][C][N]([CH3])[C][c]3[c][c][c][c][c]3  
 8001\_4897  
 Oc1c(C=Nc2ccc3c(oc4ccccc34)c2)cc(Br)cc1N(=O)=[O-]  
 8002\_9863  
 Oc1ccc(Nc2nc(cs2)c2ccc(Cl)cc2)cc1  
 8008\_8749  
 [O-]=N(=O)c1cccc(c1)C1Nc2ccc(Cl)cc2C2C=CCC12  
 8008\_4656  
 Clc1cccc1c1nnc(NC(=O)c2occc2)s1  
 K907\_0076  
 Cc1cccc1OCc1onc(n1)c1ccc(NC(=O)c2occc2)cc1  
 1910\_1439  
 Oc1c(Cl)cc(Cl)cc1C=NNC(=O)c1cccc(c1)N(=O)=[O-]  
 K647\_0156  
 Cc1cccc(Nc2nc(NCCC3=CCCC3)nc(n2)N2CCOCC2)c1

## Toxicophores

1\_2\_aminothiazole  
 s1ccnc1[\$([NX3H2&!R]),\$( [NX3H1&!R][c,C]),\$( [NX3&!R]([c,C])[c,C])]

1\_2\_dicarbonyl\_oxalyl  
 [\$([CD3&!R][#6,#8,#7,F,Cl,I,Br]),\$( [CD3&!R][#1]),\$( [CD2&!R])](=[OD1&!R])[\$([CD3&!R][#6,#8,#7,F,Cl,Br,I]),\$( [C  
 D3&!R][#1]),\$( [CD2&!R])]=[OD1&!R]

1\_2\_thiazol\_3\_one  
 S1[NX3H1]C(=[OX1])C=C1

1\_aminobenzotriazole  
 Nn1nnc2ccccc12

2\_phenylbenzimidazole  
 c2ccc3nc(c4ccccc4)[nX3H1]c3c2

3\_amino\_9\_ethylcarbazoles  
 CCN1C2=C(C=C(C=C2)N)C3=CC=CC=C31

3\_methylindole  
 C1=C([CX4H3])c2ccccc2[NX3H1]1

4\_subst\_n\_alkyltetrahydropyridines  
 [a]C1=CCN([A])CC1

4\_vinyl\_pyridine  
 c1cnccl1[CX3&!R]=[CX3&!R]

6\_membered\_aromatic\_sulfur  
 [SD2]1[#7,#6]=CC(=[OX1&!R])C=[#7,#6]1

9\_aminoacridine  
 c1cccc2c([NX3&!RH2])c3ccccc3nc12

acetal\_1\_in\_ring  
 C1([SX2&!R][#6&!R])=NCCS1

acetal\_both\_in\_ring  
 C1(=[NX2&!R][CX2&!R]#[NX1&!R])SCCS1

acetylene\_alkyne  
 [#1,#6]C#CC  
 acrylamide  
 [\$(NX3H2&!R)],\$(NX3H1&!R)[c,C],\$(NX3&!R)([c,C])[c,C])[CX3&!R](=[OX1])[CX3&!R]=[\$(CX3H2&!R)],\$(CX3H1&!R)[c,C]),\$(CX3H0&!R)([c,C])[c,C])  
 acyclic\_acetal  
 [#6][OX2&!R][\$(CX4&!RH2)],\$(CX4&!RH1)[#6]),\$(CX4&!R)([#6])[#6])[OX2&!R][#6]  
 acyclic\_acid\_halide\_acyl\_halide  
 \*[CD3&!R](F,Cl,I,Br)=[OX1]  
 acyclic\_alkyne  
 [#6][CX2&!R]#[CX2&!R][#6]  
 acyclic\_ketone  
 [#6&!R][CD3&!R](=[OD1&!R])[#6&!R]  
 acyl\_amide  
 [C,c][C;!R](=O)[N;!R][C;!R](=O)[C,c]  
 acyl\_cyanides  
 [NX1]#[CX2&!R][CX3&!R](=[OX1])[#6]  
 acyl\_hydrazone\_cyclic  
 [#6]=[NX2][NX3][CX3]=[OX1]  
 acyl\_isoamide\_aromatic  
 n1coc(=[OX1])cc1  
 adamantane  
 C1C2CC3CC1CC(C2)C3  
 aldehyde  
 [\*][CX3&!RH1]=[OD1]  
 alkyl\_halide\_noF  
 [CX4&!R][Br,I,Cl]  
 alkynes  
 [#6][#6]#[#6][#6,#1]  
 alpha\_haloamines  
 [F,Cl,I,Br][#7]  
 alphahalo\_ketone\_carbonyl  
 [#6][CD3&!c](=[OD1])[CX4&!c][Cl,Br,I,F]  
 anhydride  
 [OX1]=[CD3]([\*])[OD2][CD3](=[OX1])[\*]  
 anthracene  
 a1aa2aa3aaaaa3aa2aa1  
 arylhydroxamic\_acid  
 c[CX3](=O)[NX3H1][OX2H1]  
 azide  
 [\$(N#[N+]-[N-]),\$(N-[N+]=N)]  
 aziridine  
 N1[\$(CX4H2)],\$(CX4H1)[#6&!R]),\$(CX4)([#6&!R])[#6&!R])[\$(CX4H2)],\$(CX4H1)[#6&!R]),\$(CX4)([#6&!R])[#6&!R])]  
 azo  
 [#6][NX2]=[NX2][#6]  
 azocyanamide  
 [N;R0]=[N;R0]C#N  
 benzodioxolane  
 [CX4H2]1Oc2ccccc2O1  
 beta\_heterosubstituted\_carbonyl  
 [OD1&!R]=[\$(CD3&!R)];!\$([CD3&!R][#8])CC([F,Br,I,Cl])  
 betalactams  
 [OX1&!R]=C1CCN1C  
 carbamate\_thiocarbamate  
 [NX3&!R][CX3&!R](=[OX1,SX1])[OX2&!R,#16&!R][#6]  
 carbamic\_acid  
 [\$(NX4+)],\$(ND1&!R)],\$(NX3&!H2)],\$(NX3&!RH1)[#6]),\$(NX3&!R)([#6])[#6])[CD3&!R](=[OD1&!R])[OX2&!RH1,OX1-]  
 carbazide  
 O=\*N=[N+]=[N-]  
 carbodiimide  
 [#6][NX2]=C=[NX2][#6]  
 catechol  
 [OH]c1c([OH])cccc1  
 chloramidine  
 [Cl]C([C&R0])=N  
 coumarines  
 [OX1&!R]=c1ccc2ccccc2o1  
 crown\_2\_2  
 C[#8,#7,#16]CC[#8,#7,#16]CC[#8,#7,#16]C  
 crown\_2\_3  
 C[#8,#7,#16]CCC[#8,#7,#16]CC[#8,#7,#16]C  
 crown\_3\_3  
 C[#8,#7,#16]CCC[#8,#7,#16]CCC[#8,#7,#16]C  
 cyanohydrins  
 [ND1&!R]#[CD2&!R][CX4&!R][OD2H1]  
 cyanophosphonate  
 P(OC)(OC)(=O)C#N

cyclopropylamine  
C1CC1[NX3&!R]  
diazonium  
[c,C][N+&!R]#[N&!R]  
ellipticine  
Cc1c2[nH]c3cccc3c2c(C)c2cnccc12  
enamine  
[CX3]=[CX3&!R][NX3&!R]  
epoxide  
[OX2r3]1[#6r3][#6r3]1  
fmoc  
c12c(cccc1)c1c([CX4H1]2CO[CX3H0])(=[OX1])cccc1  
formic\_acid\_esters  
[CX3H1&!R])(=[OX1])[OX2&!R][#6]  
furan  
c1ccco1  
furocoumarines  
[OX1&!R]=c1ccc2cc3ccoc3cc2o1  
halo\_alkene  
[Br,F,I,Cl][\$( [CX3&!R][#6] ),\$( [CX3&!RH1] )]=\$( [CX3&!R]([#6])[#6] ),\$( [CX3&!RH1][#6] ),\$( [CX3&!RH2] )]  
halo\_amine  
[CX4&!R][\$( [NX3&!RH1] ),\$( [NX3&!R][#6] )][Br,F,I,Cl]  
halopyrimidine  
c1cnc([F,Cl,Br,I])nc1  
hemiaminal  
[OX2&!RH1][\$( [CX4&!RH2] ),\$( [CX4&!RH1][#6] ),\$( [CX4&!R]([#6])[#6] )][\$( [NX3&!RH2] ),\$( [NX3&!RH1][#6] ),\$( [NX3&!R]([#6])[#6] )]  
hemiketal  
[OX2&!RH1][\$( [CX4&!RH2] ),\$( [CX4&!RH1][#6] ),\$( [CX4&!R]([#6])[#6] )][\$( [OX2&!RH1] ),\$( [OX2&!R][#6] )]  
heteroatom\_heteroatom\_N\_N  
[\$([#6][NH1;!R]-[NH1;!R][#6]),\$([#6][NH1;!R]-[N;!R]([#6])[#6]),\$([#6][N;!R]([#6])-[N;!R]([#6])[#6])]  
heteroatom\_heteroatom\_N\_S  
[\$([#6][NH1;!R]-[SD2;!R][#6]),\$([#6][N;!R]([#6])-[SD2;!R][#6])]  
heteroatom\_heteroatom\_O\_N  
[\$([#6][#8;!R][NH1;!R][#6]),\$([#6][#8;!R][N;!R]([#6])[#6])]  
heteroatom\_heteroatom\_S\_O  
[#6][SD2;!R]-[#8;!R][#6]  
heteroatom\_heteroatom\_S\_S  
[#6][SD2;!R][SD2;!R][#6]  
high\_risk\_aniline  
[NX3H2&!R]c1ccccc1  
hydantoin  
[OX1]=C1[NX3H1]C(=[OX1])CN1  
hydralazine  
n1ncc2cccc2c1([NX3&!RH1][NX3&!RH2])  
hydrazide  
[NX3&!R][NX3&!R][#6X3])(=[OX1])[#6]  
hydrazine  
[#6][NX3&!RH1][NX3&!RH2]  
hydrazone  
[CX3&!R]=[NX2&!R][NX3&!R]  
hydroxamic\_acid  
[CX3&!R;\$( [H0] [#6] )](=[OD1])[#7X3;\$( [H1] )][OX2&!RH1,OX1-]  
hydroxylamine  
[c,C;!\$( [#6]=[#8] )][\$( [NX3&!RH1] ),\$( [NX3&!R][#6] )][OX2&!RH1]  
imidazole  
[#6]n1cncc1  
imide  
[C,c][C;!R](=O)[N;!R][C;!R](=O)[C,c]  
imidoyl\_halide  
[\$([CX3&!RH1]),\$( [CX3&!RH0] [#6] )](=[NX2&!R])[F,Br,I,Cl]  
imine  
[CX3]=[NX2&!R]  
isocyanate  
[OD1&!R]=[CD2&!R]=[ND2&!R][#6]  
isocyanide\_isonitrile  
[#6][#7+]#[#6-]  
isothiocyanate  
[SD1&!R]=[CD2&!R]=[ND2&!R][#6]  
lawesson\_reagent\_derivative  
[#6]P1(=S)SP(S1)(=S)[#6]  
maleimide  
C1=CC(=[OX1])NC1=[OX1]  
masked\_aniline  
[\$([n]),\$( [#7H1] ),\$( [#7H0;!\$( [NX3]=[O] ) )]c1ccccc1  
meta\_aminophenol  
c1([NX3&!R])cc([OX2&!RH1])ccc1  
michael\_acceptors\_double  
[#6]=[#6][\$( [#6]=[OX1&!R] ),\$( [#6][#7&!R] ),\$( [#6][#16!R] )]

michael\_acceptors\_triple  
[#6]#[#6][\$([#6]=[OX1&!R]),\$([#6][#7&!R]),\$([#6][#16!R])]  
mustard\_gas  
[Cl]CCSCC[Cl]  
n\_acylated\_azoles  
[#6][CX3&!R]([r5])=[OX1]  
n\_oxide  
C[N+]1(CCN(CC1)C2=C3C=CC=CC3=NC4=C(N2)C=C(C=C4)Cl)[O-]  
nitramine  
[\$([NX3][NX3&!R](=O)=O),\$( [NX3][NX3+&!R](=O)[O-]),\$( [NX3][NX3+&!R]([O-])[O-])][!#8]  
nitrile  
[ND1&!R]#[CD2!R][#6]  
nitro  
[\$([NX3&!R](=O)=O),\$( [NX3+&!R](=O)[O-]),\$( [NX3+&!R]([O-])[O-])]  
nitrobenzene  
c1ccccc1[\$([NX3&!R](=O)=O),\$( [NX3+&!R](=O)[O-]),\$( [NX3+&!R]([O-])[O-])]  
nitroso  
[OD1&!R]=[\$([ND2&!R][#6]),\$( [ND2&!R][NX3])]  
o\_thiocarbamate  
[#6][OX2&!R][CX3&!R](=[SX1])[NX3&!R][#6]  
ortho\_aminophenol  
c1([NX3&!R])c([OX2&!RH1])cccc1  
ortho\_hydroxyanilines  
c1cccc([OX2&!RH1])c1[\$([NX3&!RH2]),\$( [NX3&!RH1][#6]),\$( [NX3&!R]([#6])[#6])]  
orthonitrophenyl\_ester  
[#6][CX3&!R](=[OX1])[OX2&!R]c1ccc(\$([NX3&!R](=O)=O),\$( [NX3+&!R](=O)[O-]),\$( [NX3+&!R]([O-])[O-]))cc1  
orthoquinone  
[OD1&!R]=C1C(=[OD1&!R])C=CC=C1  
oxime  
[CX3]=[NX2][OX2H1]  
oxonium  
[O+]  
para\_aminophenol  
c1([NX3&!R])ccc([OX2&!RH1])cc1  
para\_hydroquinone  
[OH]c1ccc([OH])cc1  
para\_hydroxyanilines  
c1cc([OX2&!RH1])ccc1[\$([NX3&!RH2]),\$( [NX3&!RH1][#6]),\$( [NX3&!R]([#6])[#6])]  
para\_para\_dihydroxybiphenyl  
[OH]c1ccc(c2ccc([OH])cc2)cc1  
para\_para\_dihydroxystilbene  
[OH]c1ccc([#6!R]=[#6!R]c2ccc([OH])cc2)cc1  
paranitrophenyl\_ester  
C(=O)(C)Oc1ccc(\$([NX3&!R](=O)=O),\$( [NX3+&!R](=O)[O-]),\$( [NX3+&!R]([O-])[O-]))cc1  
pentafluorophen\_ester  
C(=O)(C)Oc1c(F)c(F)c(F)c(F)c1(F)  
perhaloketone  
[#6][CD3&!R](=[OD1&!R])[CD4&!R]([F,Br,I,Cl])([F,Br,I,Cl])[F,Br,I,Cl]  
peroxide  
[#6][#8][#8][#6]  
phenanthrene\_het  
c1cccc2c1c3c(cc2)cccc3  
phenol  
[OX2H]c1ccccc1  
phosphorane  
C=p  
phosphoric\_acid\_or\_ester  
[#6,#1][OX2&!R][PX4&!R](=[OX1])([OX2&!R][#6,#1])[OX2&!R][#6,#1]  
polyenes  
[#6]=[CX3&!R][CX3&!R]=[\$([CX3&!R][#6!R]),\$( [CX3&!RH2])]  
propiolactone  
[OX1&!R]=C1OCC1  
propiosultone  
[OX1&!R]=[SX4]1(=[OX1&!R])OCCC1  
pyrrole  
c1ccnc1  
quinone  
O=[#6]1[#6]:,[#6][#6](=O)[#6]:,[#6]1  
s\_thiocarbamate  
[#6][SX2&!R][CX3&!R](=[OX1])[NX3&!R][#6]  
sulfonate\_ester  
[#6][OD2&!R]S(=[OX1])(=[OX1])[#6,#1]  
sulfone  
[\$([#16X4&!R](=[OX1])(=[OX1])([#6])[#6]),\$( [#16X4+2&!R]([OX1-])([OX1-])([#6])[#6])]  
sulfonic\_acid  
[#6][SX4&!R](=[OX1])(=[OX1])[\$([OX2H]),\$( [OX1-])]  
sulfonic\_acid\_ester  
[#6][SX4&!R](=[OX1])(=[OX1])[\$([OX2&!R][#6,#1]),\$( [OX1-])]  
sulfonium

[SX3+]  
sulfonyl\_cyanide  
[#6][SD4&!R,SD4+2&!R](=[OD1&!R])(=[OD1&!R])[CD2&!R]#[NX1]  
sulfonyl\_halide  
[#6][#16]([F,Cl,I,Br])(=[#8])=[#8]  
sulfonyl\_urea  
[NX3H1][CX3](=[OX1])[NX3H1][SX4](=[OX1])=[OX1]  
sulfoxide  
[\$([#16X3])(=[OX1])([#6])([#6]),\$([#16X3+](OX1-))([#6])([#6]))]  
sulphanyl amino  
[#6][NX3H1][SX2H1]  
terminal\_vinyl  
[CX3H1&!R]=[CX3H2&!R]  
thiazole  
slccnc1  
thiazolidinedione  
S1C(=[OX1])[NX3H1]C(=[OX1])C1  
thioacetal  
[#6][CX4&!R]([#16&!R][#6])[#16&!R][#6]  
thioamide  
[#6][CX3&!R](=[SX1&!R])[NX3]([#6])([#6])  
thiocarbonyl\_aromatic  
[C,c]=[SX1&!RH0]  
thioester  
[OX1&!R]=[c,C][SX2]  
thioic\_acid  
[\$([CX3]([OX2H1])=S),\$([CX3]([SX2H1])=O),\$([CX3]([SX2H1])=S)]  
thioketone  
[SD1&!R]=[#6]  
thiol  
[#6][SX2H1&!R]  
thiophene  
slcccc1  
thiourea  
[\$([NX3&!RH2]),\$([NX3&!RH1][#6]),\$([NX3&!R]([#6])([#6]))][CX3&!R](=[SX1&!R])[\$([NX3&!RH2]),\$([NX3&!RH1][#6]),\$([NX3&!R]([#6])([#6]))]  
toxoflavins  
CN1C2=NC(=O)N(C(=O)C2=NC=N1)C  
triacyloxime  
C(=O)N(C(=O)OC(=O)  
triazenes  
[NX3&!R][NX2&!R]=[NX2&!R]  
triazine  
[\$([ND1&!R]),\$([NX3&!RH2]),\$([NX3&!RH1][#6]))][ND2&!R]([\$([ND1&!R]),\$([NX2&!R][#6]),\$([NX2&!RH1])]  
triazole  
[#6]n1cncn1  
triflate  
OS(=O)(=O)C(F)(F)F  
triphenyl  
clcccc1[CX4&!R](clcccc1)clcccc1

## PAINS

anil\_di\_alk\_A(478)  
[#6](-[#1])(-[#1])-[#7](-[#6](-[#1])-[#1])-[#6]:1:[#6]:[#6](:[#6](:[#6](:[#6]:1)-\$([#1]),\$([#6](-[#1])-[#1]),\$([#8]-[#6](-[#1])-[#1])))-[#7])-[#1]  
anil\_di\_alk\_B(251)  
[#6]:1:[#6]:[#6](:[#6]:[#6]:[#6]:1-[#7](-[#6;X4])-[#6;X4])-[#6]=[#6]  
anil\_di\_alk\_B\_bis(251)  
[#6]:1:[#6]:[#6](:[#6]:[#6]:1-\$([#7]),\$([#7+1]))(-[#6;X4])-[#6;X4]:[#6]:[#6]  
anil\_di\_alk\_B\_ter(251)  
[#6]:=[#6]clccc([NX3&!R]([#6])([#6])cc1  
anil\_di\_alk\_C(246)  
[#6]:1:[#6]:[#6](:[#6]:[#6]:1-[#8]-[#6;X4])-[#7](-[#6;X4])-[#6](\$([#1]),\$([#6;X4]))]  
anil\_di\_alk\_D(198)  
[#6]:1:[#6]:[#6](:[#6]:[#6]:[#6]:1-[#7](-[#6;X4])-[#6;X4])-[#6;X4]-\$([#8]-[#1]),\$([#6]=[#6]-[#1]),\$([#7]-[#6;X4]))]  
anil\_di\_alk\_E(186)  
[#6](-[#1])-[#7](-[#6](-[#1])-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-\$([#1]),\$([#6](-[#1])-[#1])))-[#6](-[#1])-\$([#1]),\$([#6]-[#1])))-[#1]-[#1]  
azo\_A(324)  
[#7;!R]=[#7]  
curcumin  
[CX3!RH1]=[CX3!RH1][CX3!R]=[OX1]  
ene\_five\_het\_A(201)  
[#6]-1(=[#6])-[#6]=[#7]-[!#6&!#1]-[#6]-1=[#8]  
ene\_rhod\_A(235)  
[#7]-1-[#6]([#16])-[#16]-[#6]([#6])-[#6]-1=[#8]



ene\_five\_het\_B\_bis(90)  
c1(=[#8&!R])[n,n+1]c[#16]c1=[#6]  
ene\_five\_het\_C(85)  
[#6]-1(-[#6](-[#6]=[#6]-[!#6&!#1]-1)=[#6])=[!#6&!#1]  
ene\_five\_het\_D(46)  
[#6]-1(=[#6])-[#6](=[#8])-[#7]-[#7]-[#6]-1=[#8]  
ene\_five\_het\_E(44)  
[#7]-[#6]=[!#6]-2-[#6](=[#8])-[#6]:1:[#6]:[#6]:[#6]:[#6]:1-[!#6&!#1]-2  
ene\_five\_het\_F(15)  
[#6]:1(:[#6]:[#6]:[#6]:[#6]:1)-[#6](-[#1])=[!#6]-3-[#6](=[#8])-[#6]:2:[#6]:[#6]:[#6]:[#6]:[#6]:2-[#16]-3  
ene\_five\_one\_A(55)  
[#6]:1-2:[#6](:[#6]:[#6]:[#6]:1)-[#6](=[#8])-[#6](=[#6])-[#6]-2=[#8]  
ene\_one\_ene\_A(57)  
[#6]=[!#6](-[!#1])-[!#6](-[!#6&!#1])-[!#6](-[!#6])-[!#1]  
ene\_one\_ester(24)  
[#6]-[#6](=[#8])-[#6](-[#1])=[#6](-[#7](-[#1])-[#6])-[#6](=[#8])-[#8]-[#6]  
ene\_one\_ester\_bis(24)  
[#6]-,:[#6](=[#8])-,:[#6](-[#1])=,:[#6](-,:[#7](-,:[#1])-,:[#6](-,:[#6](-,:[#8])-,:[#8]-,:[#6]  
ene\_one\_hal(17)  
[#6]-[#6]=[#6](-[F,C1,Br,I])-[#6](=[#8])-[#6]  
ene\_one\_hal\_bis(17)  
[#6]-,:[#6]=,:[#6](-[F,C1,Br,I])-,:[#6](=[#8])-,:[#6]  
ene\_rhod\_B(16)  
[#16]-1-[#6](=[#8])-[#7]-[#6](=[#8])-[#6]-1=[#6](-[#1])-[!#6]-[#35],\$([#6]:[#6](-[#1]):[#6](-  
[F,C1,Br,I]):[#6]:[#6]-[F,C1,Br,I]),\$([#6]:[#6](-[#1]):[#6](-[#1]):[#6]-[#16]-[#6](-[#1])-  
[#1]),\$([#6]:[#6]:[#6]:[#6]:[#6]:[#6]:[#6]:[#6]:[#6]-[#8]-[#6](-[#1])-[#1]),\$([#6]:1:[#6](-[#6](-[#1])-  
[#1]):[#7](-[#6](-[#1])-[#1]):[#6](-[#6](-[#1])-[#1]):[#6]:1])  
het\_65\_A(21)  
[#8]=[#6]-[#6]2[#6]1[#7][#6](-[#6](-[#1])-[#1])[#6][#6](-[#8]-[#1])[#7]1[#7][#6]2  
het\_6\_tetrazine(18)  
[#7]-[#6]:1:[#7]:[#7]:[#6](:\$([#7]),\$([#6]-[#1]),\$([#6]-[#7]-[#1]):\$([#7]),\$([#6]-[#7]):1)-\$([#7]-  
[#1]),\$([#8]-[#6](-[#1])-[#1])  
het\_pyridiniums\_A(39)  
[#7+]:1(:[#6]:[#6]:[!#1]:[#6]:2:[#6]:1:[#6](:[#6](-\$([#1]),\$([#7]):[#6]:[#6]:2)-[#1])-[!#6](-[#1])-  
[#1])-[#1]),\$([#8;X1]),\$([#6](-[#1])-[#1])-[#6](-[#1])=[#6](-[#1])-[#1]),\$([#6](-[#1])-[#1])-[#6](-[#1])-  
[#1]-[#8]-[#1]),\$([#6](-[#1])-[#1])-[#6](-[#1])-[#6](-[#1])-[#6](-[#1])-[#6](-[#1])-[#6](-[#1])-  
[#6]:[#6]),\$([#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#1])  
hzone\_acyl\_naphthol(22)  
[#6]:1:2:[#6](:[#6](:[#6](:[#6]:1:[#6](:[#6](:[#6](:[#6]:2-[#1])-[#8]-[#1])-[#6]([#8]-[#7](-[#1])-  
[#7]=[#6]-[#1])-[#1])-[#1])-[#1])  
hzone\_anil\_di\_alk(35)  
[#6](-[#1])-[#1])-[#7](-[#6](-[#1])-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#6](-  
[#1])-[#7]-[#7]-[#6](-[#6](-[#1])-[#1])-[#16]-[#6]:[#7]),\$([#6]([#8])-[#6](-[#1])-[#1])-  
[!#1]:[!#1]:[#7]),\$([#6]([#8])-[#6]:[#6]-[#8]-[#1]),\$([#6]:[#7]),\$([#6](-[#1])-[#1])-[#6](-[#1])-[#8]-  
[#1])-[#1])-[#1])  
hzone\_enamin(30)  
[#7](-[#1])-[#7]=[#6]-[#6](-\$([#1]),\$([#6]))=[#6](-[#6])-[!#6](\$([#7]),\$([#8]-[#1]))  
hzone\_enamin\_bis(30)  
[#7](-[#1])-,:[#7]=,:[#6]-,:[#6](-\$([#1]),\$([#6]))=,:[#6](:,-[#6])-[!#6](\$([#7]),\$([#8]-[#1]))  
hzone\_enamin\_ter(30)  
[NX3&!RH1][NX2&!R]=[#6][#6]:,[#6]([OX2&!RH1])[#6]  
hzone\_pipzn(79)  
[#6]-[#7]-1-[#6](-[#1])-[#6](-[#1])-[#6](-[#1])-[#7](-[#6](-[#1])-[#1])-[#6]-1(-[#1])-[#1])-[#7]=[#6](-  
[#1])-[#6]:[!#1]  
hzone\_pyrrrol(64)  
[#7]1(-[#6])[#6]([#6](-[#1])[#6]([#6]1-[#6]=[#7]-[#7])-[#1])-[#1]  
imidazole\_A(19)  
[#7]:1:[#6](:[#7](:[#6](:[#6]:1-[#6]:2:[#6]:[#6]:[#6]:[#6]:[#6]:2)-[#6]:3:[#6]:[#6]:[#6]:[#6]:3)-[#1])-  
[#6]:[!#1]  
imine\_one\_fives(89)  
[#6]-1=[!#1]-[!#6&!#1]-[#6](-[#6]-1=[!#6&!#1;!R])=[#8]  
imine\_one\_sixes(27)  
[#6]-1(-[#6]([#8])-[#7]-[#6]([#8])-[#7]-[#6]-1=[#8])=[#7]  
keto\_keto\_beta\_A(68)  
[#6]:1-2:[#6](:[#6]:[#6]:[#6]:1)-[#6]([#8])-[#6;X4]-[#6]-2=[#8]  
naphth\_amino\_A(25)  
[#6]:2:[#6]:1:[#6]:[#6]:[#6]:[#6]-3:[#6]:1:[#6](:[#6]:[#6]:2)-[#7]-[#6]=[#7]-3  
naphth\_amino\_A\_bis(25)  
[#6]:2:[#6]:1:[#6]:[#6]:[#6]:[#6]:3:[#6]:1:[#6](:[#6]:[#6]:2):[#7]:[#6]:[#7]:3  
naphth\_amino\_B(25)  
[#6]:2:[#6]:1:[#6]:[#6]:[#6]:[#6]-3:[#6]:1:[#6](:[#6]:[#6]:2)-[#7](-[#6;X4]-[#7]-3-[#1])-[#1]  
pyrrole\_A(118)  
[#7]2(-[#6]:1:[!#1]:[#6]:[#6]:[#6]:[#6]:1)[#6]([#6][#6]([#6]2-[#6;X4])-[#1])-[#6;X4]  
pyrrole\_B(29)  
[#7]2(-[#6]:1:[!#1]:[#6]:[#6]:[#6]:[#6]:1)[#6]([#6][#6]([#6]2-[#6]:[#6])-[#1])-[#6;X4]  
rhod\_sat\_A(33)  
[#7]-1-[#6]([#16])-[#16]-[#6;X4]-[#6]-1=[#8]  
sulfonamide\_A(43)

[#6]:1(:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#8]-[#1])-[F,Cl,Br,I]-[#1])-[F,Cl,Br,I]-[#1])-[#16](=[#8])(=[#8])-[#7])  
sulfonamide\_B(41)  
[#6]:1:[#6]:[#6](:[#6]:[#6]:[#6]:1-[#8]-[#1])-[#7](-[#1])-[#16](=[#8])=[#8]  
thiaz\_ene\_A(128)  
[#6]-1(=[#6](-[#1])-[#1]),\$([#6](-[#1])-[#1]),\$([#6]=[#8]))-[#16]-[#6](-[#7]-1-[\$([#1]),\$([#6]-[#1]),\$([#6]:[#6])])=[#7;!R)]-[\$([#6](-[#1])-[#1]),\$([#6]:[#6])]  
thiaz\_ene\_A\_bis(128)  
[#6]:1(:[#6](-[\$([#1]),\$([#6](-[#1])-[#1]),\$([#6]=[#8])])]:[#16]:[#6](:[#7]:1-[\$([#1]),\$([#6]-[#1]),\$([#6]:[#6])])=[#7;!R)]-[\$([#6](-[#1])-[#1]),\$([#6]:[#6])]  
thiaz\_ene\_B(17)  
[#6]-1(=[#6](-!@[#6]([#6]=[#8])-[#7]-[#6](-[#1])-[#1])-[#16]-[#6](-[#7]-1-[\$([#6](-[#1])-[#1])-[#6](-[#1])-[#6](-[#1])-[#1])-[#1]),\$([#6]:[#6])])=[#16])-[#7]-[#6]([#8])-[#6]:[#6]),\$([#7](-[#1])-[#1])]  
thiaz\_ene\_B\_bis(17)  
[#7]1(\$([#6]:[#6]),\$([#6H2][#6H1]=[#6H2]))[#6]([#16])[#16][#6]([#6&!R]([#8])[#7][#6H2])=,:[#6]1[\$([#7H2]),\$([#7][#6]([#8])[#6]:[#6])]  
thio\_carbonate\_A(15)  
[#8]-1-!#6](-[#16]-[#6]:2:[#6]-1:[#6]:[#6]:[#6](:[#6]:2)-[\$([#7]),\$([#8])])=[\$([#8]),\$([#16])]  
thio\_carbonate\_A\_bis(15)  
[#8]1[#6]([#16]c2c1ccc(c2)[\$([#7]),\$([#8])])=[\$([#8]),\$([#16])]  
thio\_dibenzo(23)  
[#16]=[#6]-1-!#6]=,:[#6]-!#6&!#1]-[#6]=,:[#6]-1  
thio\_dibenzo\_bis(23)  
S=c1cc(n(c(c1)C)C)cc1occc1C  
thio\_ketone(43)  
[#6][#6]([#16])[#6]  
thiophene\_amino\_Aa(45)  
[#7](-[#1])-[#1]-[#6]:1:[#6](:[#6](:[#6](:s:1)-!#1)-!#1)-[#6]=[#8]  
thiophene\_amino\_Ab(40)  
[\$([#1]),\$([#6](-[#1])-[#1]),\$([#6]:[#6])]-[#6]:1:[#6](:[#6](:[#6](:s:1)-[#7](-[#1])-[#6]([#8])-[#6])-[#6]([#8])-[#8])-[#6]:1:[#6]:[#6]:[#6]:[#6]:1),\$([#6]:1:[#16]:[#6]:[#6]:[#6]:1)]  
thiophene\_hydroxy(28)  
s1[#6][#6][#6]([#6]1)-[#8]-[#1]

acyl\_het\_A(9)  
[#7+](:[#1]:[#1]:[#1])-[#1]=[#8]  
acyl\_het\_A\_bis(9)  
[#7+](:[#1]:[#1]:[#1])[#1]=[#8]  
amino\_acridine\_A(1)  
[#6]:1:[#6]:[#6]:[#6]:2:[#6]:1:[#6]:[#6]:3:[#6](:[#7]:2):[#7]:[#6]:4:[#6](:[#6]:3-[#7]):[#6]:[#6]:[#6]:4  
anil\_NH\_alk\_A(5)  
[#6]:1(:[#6](:[#6]-2:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#7](-[#6](-[#7]-2-[#1])=[#8])-[#1])-[#1])-[#7](-[#1])-[#6](-[#1])-[#1])  
anil\_NH\_alk\_B(3)  
[#7](-[#1])-[#6]:1:[#6]:[#6]:!#1:[#6]:[#6]:1)-[#6]:2:[#6]:[#6]:[#6](:[#6]:[#6]:2)-[#7](-[#1])-[#6]-[#1]  
anil\_NH\_alk\_C(2)  
[#6](-[#1])-[#7](-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#1])-[#7](-[#1])-[#6]-[#1])  
anil\_NH\_alk\_D(2)  
[#7](-[#1])-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6]:1-[#7](-[#1])-[#6](-[#1])-[#6](-[#1])-[#6](-[#1])-[#6](-[#1])-[#1])-[#1])-[#1])-[#1])  
anil\_NH\_no\_alk\_A(1)  
[#7]:1:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#7](-[#1])-[#1])-[#1])-[#7](-[#1])-[#6]:[#6]  
anil\_NH\_no\_alk\_B(1)  
[#7](-[#1])-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#7](-[#1])-[#16]([#8])=[#8])-[#1])-[#7](-[#1])-[#6](-[#1])-[#1])-[F,Cl,Br,I]-[#1])  
anil\_OC\_alk\_A(4)  
[#6]:1:2:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#1])-[#1])o:[#6]:3:[#6](-[#1]):[#6](:[#6](-[#8]-[#6](-[#1])-[#1]):[#6](:[#6]:2:3)-[#1])-[#7](-[#1])-[#6](-[#1])-[#1])  
anil\_OC\_alk\_B(3)  
[#6]:1:3:[#6](:[#6]:[#6]:[#6]:1)-[#7]-2-[#6]([#8])-[#6]([#6](-[F,Cl,Br,I]-[#6]-2=[#8])-[#7](-[#1])-[#6]:[#6]:[#6]:3  
anil\_OC\_alk\_C(3)  
[\$([#1]),\$([#6](-[#1])-[#1])]-[#8]-[#6]:1:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#1])-[#1])-[#7](-[#1])-[#6](-[#1])-[#1])-[#6]:2:[#7]:[#6]:[#6]:[#7]:2  
anil\_OC\_alk\_D(2)  
[#6](-[#1])-[#1])-[#8]-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#6](-[#1])-[#1])-[#1])-[#7](-[#1])-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])  
anil\_OC\_alk\_E(1)  
[#6](-[#1])-[#1])-[#8]-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#1])-[#1])-[#7](-[#1])-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])  
anil\_OC\_alk\_F(1)  
[#6](-[#1])-[#1])-[#8]-[#6]:1:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#1])-[#1])-[#7](-[#1])-[#6](-[#1])-[#6]([#8])-[#16]  
anil\_OC\_no\_alk\_A(8)  
[#7](-[#1])-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#7]:[#6]:1-[#1])-[#8]-[#6]:2:[#6]:[#6]:[#6]:[#6]:[#6]:2)-[#1])-[#1]  
anil\_OC\_no\_alk\_B(4)

[#6]:1:[#6](:[#6]:2:[#6](:[#6]:[#6]:1):[#6]:[#6]:[#6]:[#6]:2)-[#8]-[#6]:3:[#6](:[#6](:[#6](:[#6](:[#6]:3-  
[#1])-[#1])-[#7]-[#1])-[#1])-[#1]  
anil\_OC\_no\_alk\_C(3)  
[#7](-[#1])(-[#1])-[#6]:1:[#6](:[#6]:[#6]:[#6]:[#6]:1)-[#8]-[#6](-[#1])(-[#1])-[#6]:[#6]  
anil\_OH\_alk\_A(8)  
[#6]:1:[#6](:[#6]:[#6]:[#6]:1)-[#6](-[#1])(-[#1])-[#7](-[#1])-[#6]:2:[#6](:[#6](:[#6](:[#6]:2-  
[#1])-[#1])-[#8]-[#1])-[#1])-[#1]  
anil\_OH\_no\_alk\_A(1)  
[#7](-[#1])(-[#1])-[#6]:1:[#6]:[#6]:[#6](:[#6]:[#6]:1-[#8]-[#1])-[#16](=[#8])(=[#8])-[#8]-[#1]  
anil\_OH\_no\_alk\_B(1)  
[#6]:2(:[#6]:1:[#6](:[#6](:[#6](:[#6]:1:[#6](:[#6](:[#6]:2-[#8]-[#1])-[#6]=[#8])-[#1])-[#1])-[#1])-  
[#1])-[#1])-[#7](-[#1])-[#1]  
anil\_alk\_A(1)  
[#6](-[#1])(-[#1])-[#8]-[#6]:[#6]-[#6](-[#1])(-[#1])-[#7](-[#1])-  
[#6]:2:[#6](:[#6](:[#6]:1:[#7](:[#6](:[#7]:[#6]:1:[#6]:2-[#1])-[#1])-[#6]-[#1])-[#1])-[#1]  
anil\_alk\_B(1)  
[#7](-[#1])(-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#6](-[#1])-[#1])-[#1])-[#6](-[#1])(-  
[#1])-[#6](-[#1])(-[#1])-[#6]:2:[#6](:[#6](:[#6](:[#6](:[#6]:2-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#1])-[#1]  
anil\_alk\_C(1)  
[#7](-[#1])(-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#6](-[#6])(-[#6])-[#6]:2:[#6](:[#6](:[#6](:[#6]:2-  
[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#1])-[#1]  
anil\_alk\_D(1)  
[#7](-[#1])(-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#6](-[#1])(-[#6](-[#1])-[#1])-[#6](-[#1])-  
[#1])-[#1])-[#1])-[#6](-[#1])(-[#1])-[#6](-[#1])(-[#1])-[#7](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1]  
anil\_alk\_bim(9)  
[#6]:1:3:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#7](-[#1])-[#6](-[#1])(-[#1])-  
[#6]:2:[#6]:[#6]:[#6]:[#6]:2)-[#1]:[#7]:[#6](-[#1]):[#7]:3-[#6]  
anil\_alk\_indane(1)  
[#6]:1:3:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#7](-[#1])-[#6](-[#1])(-[#1])-  
[#6]:2:[#6]:[#6]:[#6]:[#6]:2)-[#1]:[#7]:[#6](-[#1]):[#7]:3-[#6]  
anil\_alk\_indane(1)  
[#6]:1:3:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#7](-[#1])-[#6](-[#1])(-[#1])-  
[#6]:2:[#6]:[#6]:[#6]:[#6]:2)-[#6]-[#6]-3-4)-[#6;X4]  
anil\_alk\_thio(4)  
[#6]-1-3=[#6](-[#6](-[#7]-[#6]:2:[#6]:[#6]:[#6]:[#6]-1:2)(-[#6])-[#6]-[#16]-[#16]-[#6]-3=[!#1]  
anil\_alk\_thio\_bis(4)  
c13c(-[#6](-[#7]-c2cccc12)(-[#6])-[#6])ssc3=[!#1]  
anil\_di\_alk\_F(14)  
[#6]:1:[#6]:[#6](:[#6]:[#6]:[#6]:1-[#6;X4]-[#6]:2:[#6]:[#6]:[#6](:[#6]:[#6]:2)-[#7](-[#6](\$([#1]),\$([#6;X4]))-  
[\$([#1]),\$([#6;X4]))]-[#7](-[#6](\$([#1]),\$([#6;X4])))-[#6](\$([#1]),\$([#6;X4]))]  
anil\_di\_alk\_G(9)  
[#6;X4]-[#7](-[#6;X4])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#6]2=,:[#7][#6]:[#6]:[!#1]2)-[#1])-  
[#1]  
anil\_di\_alk\_H(6)  
[#6]:1(:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#7](-[#1])-[#16])(=[#8])(=[#8])-[#6]:2:[#6]:[!#1]:[#6]:[#6]:[#6]:2)-  
[#1])-[#7](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#1])-[#1]  
anil\_di\_alk\_I(4)  
[#6]:1(:[#6](:[#6](:[#6](:[#6]:1-[#7](-[#1])-[#6]([#8])-[#6]:2:[#6]:[#6]:[#6]:[#6]:2)-[#1])-  
[#7](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#1])-[#1]  
anil\_di\_alk\_J(3)  
[#6](-[#1])(-[#1])-[#7](-[#6](-[#1])-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#6](-  
[#1])=[#7]-[#7]=[#6](-[#6])-[#6]:[#6](-[#1])-[#1]  
anil\_di\_alk\_K(2)  
[#6]:1:[#6]:[#6](:[#6]:[#6]:[#6]:1-[#7](-[#1])-[#1])-[#7](-[#6;X3])-[#6;X3]  
anil\_di\_alk\_L(1)  
[#6]:1:[#6]:[#6]:[#6]-2:[#6](:[#6]:1)-[#6](-[#6](-[#7]-2-[#6](-[#1])(-[#1])-[#6](-[#1])(-[#1])-[#7]-4-[#6](-  
[#6]:3:[#6]:[#6]:[#6]:[#6]:3-[#6]-4=[#8])=[#8](-[#1])-[#1])-[#1])-[#1]  
anil\_di\_alk\_M(1)  
[#6]:1(:[#6]:4:[#6](:[#7]:[#6](:[#6]:1-[#6](-[#1])(-[#1])-[#7]-3-[#6]:2:[#6](:[#6](:[#6](:[#6]:2-[#6](-  
[#1])(-[#1])-[#6]-3(-[#1])-[#1])-[#1])-[#1])-[#1])-[#1]:[#6](:[#6](:[#6](:[#6]:4-[#1])-[#1])-[#1])-  
[#1])-[#1]  
anil\_di\_alk\_N(1)  
[#6]:1-2:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#1])-[#6]([#6](-[#1])-[#6]-3-[#6](-[#6]#[#7])-  
[#6](-[#1])-[#6](-[#1])-[#6](-[#1])-[#7]-2-3)-[#1]  
anil\_di\_alk\_O(1)  
[#6]:1(:[#6](:[#6](:[#6](:[#6]:1-[#7](-[#1])-[#6]([#16])-[#7](-[#1])-  
[#6]:2:[#6]:[#6]:[#6]:2)-[#1])-[#7](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#1])-[#1]  
anil\_di\_alk\_P(1)  
[#6](-[#1])(-[#1])-[#7](-[#6](-[#1])-[#1])-[#6]:2:[#6]:[#6]:[#6]:1:s:[#6](:[#7]:[#6]:1:[#6]:2)-[#16]-[#6](-  
[#1])-[#1]  
anil\_di\_alk\_coum(1)  
[#6]:1:[#6](:[#6]:[#6]:[#6]:1)-[#7](-[#6]-[#1])-[#6](-[#1])-[#6](-[#1])-[#6](-[#1])-[#7](-[#1])-  
[#6]([#8])-[#6]-2-[#6](-[#8]-[#6](-[#6]([#6]-2-[#6](-[#1])-[#1])-[#1])=[#8])-[#6](-[#1])-[#1]  
anil\_di\_alk\_dhp(1)  
[#7]-2-[#6]=[#6](-[#6]=[#8])-[#6](-[#6]:1:[#6]:[#6]:[#6](:[#6]:[#6]:1)-[#7](-[#6](-[#1])-[#1])-[#6](-[#1])-  
[#1])-[#6]~3=[#6]-2~[#7]~[#6]~[#16]~[#7]~[#6]~3~[#7]  
anil\_di\_alk\_ene\_A(8)  
[#6](-[#1])(-[#1])-[#7](-[#6](-[#1])-[#1])-[#6]-2=[#6](-[#1])-[#6]:1:[#6](:[#6]:[#6]:[#6]:1)-[#16;X2]-  
[#6]:3:[#6]-2:[#6]:[#6]:[#6]:3  
anil\_di\_alk\_ene\_B(4)  
[#6](-[#1])(-[#1])-[#7](-[#6](-[#1])-[#1])-[#6]-2=[#6]-[#6]:1:[#6](:[#6]:[#6]:[#6]:1)-[#6]-2(-[#1])-[#1]  
anil\_di\_alk\_furan\_B(2)

$[#6](-[#1])(-[#1])-[#7](-[#6](-[#1])-[#1])-[#6]:1:[#6](-[#1]):[#6](:[#6](\circ:1)-[#6](-[#1])=[#6]-[#6]#[#7])-[#1]$   
 $anil\_di\_alk\_indol(1)$   
 $[#6]:1:2:[#6](:[#6](:[#6](:[#6](:[#6]:1-#[#1])-[#1])-[#7](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#1]):[#6](:[#6](-[#1]):[#7]:2-#[#1])-[#16](=[#8])=[#8]$   
 $anil\_no\_alk\_A(1)$   
 $[#7](-[#1])(-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-#[#7]=[#6]-2-#[6](=[#6]-[#6]-[#6]=[#6]-2)-#[#1])-[#1])-[#1])-[#1])-[#1]$   
 $anil\_no\_alk\_B(1)$   
 $[#7](-[#1])(-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-#[7]:2:[#6]:[#6]:[#6]:[#6]:2)-#[#1])-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#1]$   
 $anil\_no\_alk\_C(1)$   
 $[#7](-[#1])(-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-#[#1])-[#1])-[#6]:2:[#6](-[#1]):[#6](:[#6](-[#6](-[#1])-[#1]):\circ:2)-[#6]=[#8])-[#1])-[#1]$   
 $anil\_no\_alk\_D(1)$   
 $[#7]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-#[7](-[#1])-[#1])-[#6](-[#1])-[#1])-[#1])-[#6](-[#1])-[#1])-[#7](-[#1])-[#1]$   
 $anil\_no\_alk\_indol\_A(1)$   
 $[#6]:1:2:[#6](:[#6](:[#6](:[#6](:[#6]:1-#[#1])-[#1])-[#7](-[#1])-[#1])-[#1]):[#6](:[#6](-[#1]):[#7]:2-#[6](-[#1])-[#1])-[#1]$   
 $anisol\_A(5)$   
 $[#6]:1(:[#6](:[#6](:[#6](:[#6](:[#6]:1-#[#1]),\$(#[6](-[#1])-[#1]))-#[#1])-[#8]-[#6](-[#1])-[#1])-[#6](-[#1])(-[#1])-[#6]([#7](-[#1])-[#6](=[#8])-[#6](-[#1])-[#1])-[#6](-[#1])-[#1]),\$(#[6](-[#1])(-[#1])(-[#1])-[#1])-[#7](-[#1])-[#6](=[#16])-[#7](-[#1])-[#1])-[#1])-[#8]-[#6](-[#1])-[#1]$   
 $anisol\_B(2)$   
 $[#6](-[#1])(-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-#[8]-[#6](-[#1])-[#1])-[#1])-[#1])-[#6](-[#1])-[#1])-[#7](-[#1])-[#6];X4)-#[1]$   
 $anthranil\_acid\_B(3)$   
 $[#6]:1:[#6]-3:[#6](:[#6](:[#6]:1-#[6](=[#8])-[#7](-[#1])-[#6]:2:[#6](:[#6]:[#6]:[#6]:2)-[#6](=[#8])-[#6](-[#6]-1),\$([#8]-[#1]))-[#6](-[#7](-[#6]-3=[#8])-[#6](-[#1])-[#1])=[#8]$   
 $anthranil\_acid\_C(2)$   
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 $anthranil\_acid\_D(2)$   
 $[#6]:12:[#6](:[#6]:[#6]:[#6]:[#7]:1)[#6]([#6](-[#6]([#6](-[#6]([#6](-[#6](-[#1])-[#1])-[#1])-[#6]([#8])-[#6](-[#6]-1)),\$([#8]-[#1]))-#[7](-[#1])-[#6]:1:[#6]:[#6]:[#6]:[#6]:1-#[6](=[#8])-[#6](-[#6]-1),\$([#8]-[#1]))-[#7]=[#6](-[#6]:2:[#6]:[#6]:[#6]:[#6]:2)-[#8]-3$   
 $anthranil\_acid\_E(2)$   
 $[#6]:1(:[#6]:[#6]:[#6]:1-#[7](-[#1])-[#6]([#8])-[#6]:[#6]-[#6]([#8])-[#6](-[#6]-1),\$([#8]-[#1]))-[#8]-[#1]$   
 $anthranil\_acid\_F(2)$   
 $[#6]:1(:[#6]:[#6]:[#6]:1-#[7](-[#1])-[#6]([#8])-[#6]:[#6]-[#6]([#8])-[#6](-[#6]-1),\$([#8]-[#1]))-[#8]-[#1]$   
 $anthranil\_acid\_G(1)$   
 $[#6]:1(:[#6]:[#6]:[#6](:[#6](:[#6]:1-#[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#1])-[#6]([#8])-[#6](-[#6]-1),\$([#8]-[#1]))-[#7](-[#1])-[#6]:[#6]$   
 $anthranil\_acid\_H(1)$   
 $[#6]:1:[#6](:[#6]:2:[#6]:[#6]:[#6]:1)[#6]([#6]([#7]2-#[#1])-[#6]:[#6]-[#6]:[#6]-[#6]([#8])-[#6](-[#6]-1),\$([#8]-[#1]))$   
 $anthranil\_acid\_I(1)$   
 $[#6]:1:2(:[#6](:[#6](:[#6](:\circ:1)-[#6])-[#1])-[#1])-[#6]([#8])-[#7](-[#1])-[#6]:[#6](-[#1]):[#6](-[#1]):[#6](-[#1]):[#6]:2-#[6]([#8])-[#6](-[#6]-1),\$([#8]-[#1]))$   
 $anthranil\_acid\_J(1)$   
 $[#7](-[#1])(-[#1])-[#6]:1:[#6](-[#6]([#8])-[#6](-[#6]-1),\$([#8]-[#1])): [#6]:[#6]:[#6](:[#7]:1)-[#6]:[#6]$   
 $anthranil\_amide\_A(1)$   
 $[#6]:1:[#6](:[#6]:[#6]:[#6]:1-#[6]([#8])-[#7](-[#1])-[#6]:2:[#6](:[#6]:[#6]:[#6]:2)-#[6]([#8])-[#7](-[#1])-[#7](-[#1])-[#6]:3:[#7]:[#6]:[#6]:s:3$   
 $azulene(4)$   
 $[#6]:2:[#6]:[#6]:1:[#6](:[#6]:[#6]:[#6]:1):[#6]:[#6]:2$   
 $colchicine\_A(3)$   
 $[#6]-1(-[#6]([#6]-[#6]=[#6]-[#6]=[#6]-1)-[#7]-[#1])=[#7]-[#6]$   
 $colchicine\_B(1)$   
 $[#6]:1(:[#6]:[#6]:[#6](:[#6]:[#6]:1)-[#6]-3=[#6]-[#6](-[#6]2[#6]o[#6]#[6]2-#[6]([#6]-3)-[#8]-[#1])=[#8])-[#16]-[#6](-[#1])-[#1]$   
 $colchicine\_het(1)$   
 $[#6]:1-3:[#6](:[#6]:[#6]:[#6]:1)-[#16]-[#6]([#7]-[#7]=[#6]-2-#[6]=[#6]-[#6]=[#6]-[#6]=[#6]-2)-[#7]-3-#[6](-[#1])-[#1]$   
 $coumarin\_A(2)$   
 $[#6]:1-3:[#6](:[#6](:[#6](:[#6](:[#6]:1)-[#8]-[#6]-[#1])-[#1])-[#1])-[#6]:2:[#6](:[#6](:[#6](:[#6]:2-#[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#6]([#8])-[#8]-3$   
 $coumarin\_B(2)$   
 $[#6]:1-2:[#6](:[#6]:[#6]:[#6]:1-#[6](-[#1])-[#1])-[#6](-[#1])=[#6](-[#1])-[#1])-[#6]([#8])-[#7](-[#1])-[#6]:[#6]-[#6]([#8])-[#8]-2)-[#1]$   
 $coumarin\_C(1)$   
 $[#6]-2(-[#6]([#7]-[#6]:1:[#6]:[#6](:[#6]:[#6]:1-#[8]-2)-[C1])=[#8]$   
 $coumarin\_D(1)$   
 $[#6]:1:[#6]:[#6](:[#6]:[#6]-2:[#6]:1-#[6]([#6](-[#1])-[#6]([#8])-[#8]-2)-[#6]:3:[#6]:[#6]:[#6]:3)-[#8]-[#6](-[#1])-[#1])-[#6]:[#8]:[#6]$   
 $coumarin\_E(1)$   
 $[#6]:1-3:[#6](:[#6]:2:[#6](:[#6]:[#6]:1-[Br]):\circ:[#6]:[#6]:2-#[6]([#6]-[#6]([#8])-[#8]-3)-[#1]$   
 $coumarin\_F(1)$

[#6]:1-3:[#6](:[#6]:[#6]:[#6]:[#6]:1)-[#6](=[#6](-[#6]([#8]-[#7](-[#1])-[#6]:2:[#7]:o:[#6]:[#6]:2-[Br])-[#6]([#8])-[#8]-3)-[#1])  
coumarin\_G(1)  
[#6]:1-2:[#6](:[#6]:[#6](:[#6]:[#6]:1-[F,Cl,Br,I])-[F,Cl,Br,I])-[#6]([#6](-[#6]([#8]-[#7](-[#1])-[#1])-[#6]([#7]-[#1])-[#8]-2)-[#1])  
coumarin\_H(1)  
[#6]:1-3:[#6](:[#6]:[#6]:[#6]:[#6]:1)-[#6]([#6](-[#6]([#8]-[#7](-[#1])-[#6]:2:[#7]:[#6](:[#6]:s:2)-[#6]:[#16]:[#6]-[#1])-[#6]([#8])-[#8]-3)-[#1])  
cyanamide\_A(1)  
[#8]-[#6]([#8])-[#6](-[#1])-[#1]-[#16;X2]-[#6]([#7]-[#6]#[#7])-[#7](-[#1])-[#6]:1:[#6]:[#6]:[#6]:[#6]:1  
cyano\_amino\_het\_A(1)  
[#6]:1(:[#6](:[#6]:2:[#6](:[#7]:[#6]:1-[#7](-[#1])-[#1]):[#6]:[#6]:[#6](:[#6]:2-[#7](-[#1])-[#1])-[#6]#[#7])-[#6]#[#7])-[#6]#[#7])  
cyano\_amino\_het\_B(1)  
[#7]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#16;X2]-[#6]:2:[#6]:[#6]:[#6]:[#6]:2-[#7](-[#1])-[#1])-[#6]#[#7])-[#6]:3:[#6]:[#6]:[#6]:[#6]:3)-[#6]#[#7])-[#7](-[#1])-[#1])  
cyano\_cyano\_B(3)  
[#6]-1(-[#6]#[#7])(-[#6]#[#7])-[#6](-[#1])(-[#6]([#8]-[#6])-[#6]-1-[#1])  
cyano\_ene\_amine\_B(4)  
[#6]#[#6]-[#6](-[#6]#[#7])(-[#6]#[#7])-[#6](-[#6]#[#7])=[#6]-[#7](-[#1])-[#1])  
cyano\_ene\_amine\_C(3)  
[#6]:[#6]-[#6]([#8])-[#7](-[#1])-[#6]([#8])-[#6](-[#6]#[#7])=[#6](-[#1])-[#7](-[#1])-[#6]:[#6]  
cyano\_imine\_C(12)  
[#8]=[#16]([#8])-[#6](-[#6]#[#7])=[#7]-[#7]-[#1])  
cyano\_imine\_D(1)  
[#8]=[#6]-1-[#6]([#7]-[#7]-[#6]-[#6]-1)-[#6]#[#7])  
cyano\_keto\_A(2)  
[#6](-[#1])(-[#1])-[#6](-[#1])(-[#6]#[#7])-[#6]([#8])-[#6]  
cyano\_misc\_A(1)  
[#6]:2(:[#6]:1:[#6]:[#6]:[#6]:[#6]:1:[#7]:[#7]:[#6]:2)-[#6](-[#6]:[#6])-[#6]#[#7])  
cyano\_pyridone\_C(11)  
[#6]-1(-[#6]([#6](-[#6]#[#7])-[#6]([#8])~[#7]~[#6]-1-[#8])-[#6](-[#1])-[#1])=[#6](-[#1])-[#6]:[#6]  
cyano\_pyridone\_D(5)  
[#8]=[#6]-1-[#6]([#6]-[#6]([#7]-[#7]-1)-[#6]([#8])-[#6]#[#7])  
cyano\_pyridone\_E(4)  
[!#1]:[#6]-[#6]-1=[#6](-[#1])-[#6]([#6](-[#6]#[#7])-[#6]([#8])-[#7]-1-[#1])-[#6]:[#8]  
cyano\_pyridone\_F(3)  
[#7]-2(-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#6]([#8])-[#6]([#6]-[#6]([#7]-2)-[#6]#[#7])-[#6]#[#7])  
cyano\_pyridone\_G(1)  
[#7]-2(-[#6]:1:[#6]:[#6]:[#6](:[#6]:[#6]:1)-[#8]-[#6](-[#1])-[#1])-[#6]([#8])-[#6]([#6]-[#6]([#7]-2)-[#7]:3:[#6]:[#7]:[#6]:[#6]:3)-[#6]#[#7])  
dhp\_amidine\_A(1)  
[#7]-1(-[#1])-[#7]=[#6](-[#7]-[#1])-[#16]-[#6]([#6]-1-[#6]:[#6])-[#6]:[#6]  
dhp\_amino\_CN\_A(13)  
[#7](-[#1])(-[#1])-[#6]-1=[#6](-[#6]#[#7])-[#6](-[#1])(-[#6]:[#6])-[#6]([#6](-[#6]=[#6])-[#8]-1)-[#6](-[#1])-[#1])  
dhp\_amino\_CN\_B(9)  
[!\$([#7](-[#1])-[#1]),\$([#8]-[#1])]-[#6]-2=[#6](-[#6]#[#7])-[#6](-[#1])(-[#6]:[#6])-[#6]:1:[#6](:[#7](-[#6]:[#7]:[#6]:1)-[#8]-2  
dhp\_amino\_CN\_C(7)  
[#7](-[#1])(-[#1])-[#6]-1=[#6](-[#6]#[#7])-[#6](-[#1])(-[#6]:[#6])-[#6]([#6](-[#6]:[#6])-[#8]-1)-[#6]#[#7])  
dhp\_amino\_CN\_D(5)  
[#7](-[#1])(-[#1])-[#6]-2=[#6](-[#6]#[#7])-[#6](-[#1])(-[#6]:[#6])-[#6]:1:[#6](:[#6]:[#6]:s:1)-[#8]-2  
dhp\_amino\_CN\_E(4)  
[#6](-[#1])(-[#1])-[#16;X2]-[#6]-1=[#6](-[#6]#[#7])-[#6](-[#1])(-[#6]:[#6])-[#6](-[#6]#[#7])-[#6]([#8])-[#7]-1  
dhp\_amino\_CN\_F(3)  
[#7](-[#1])(-[#1])-[#6]-2=[#6](-[#6]#[#7])-[#6](-[#1])(-[#6]:1:[#6]:[#6]:s:1)-[#6]([#6](-[#6](-[#1])-[#1])-[#8]-2)-[#6]([#8])-[#8]-[#6]  
dhp\_amino\_CN\_G(1)  
[#16;X2]-1-[#6]=[#6](-[#6]#[#7])-[#6](-[#6])(-[#6]=[#8])-[#6]([#6]-1-[#7](-[#1])-[#1])-[#6]([#6]=[#8]),\$([#6]#[#7])  
dhp\_amino\_CN\_H(1)  
[#7](-[#1])(-[#1])-[#6]-1=[#6](-[#6]#[#7])-[#6](-[#1])(-[#6]:[#6])-[#16]-[#6;X4]-[#16]-1  
dhp\_keto\_A(9)  
[#7]-1(-\$([#6;X4]),\$([#1]))-[#6]=,\$([#6](-[#6]([#6]-[#6]:[#6]:[#6])-[#6](-[#6])-[#6]([#6]-1-[#6](-[#1])-[#1])-[#1])-[#6](\$([#6]=[#8]),\$([#6]#[#7]))  
diazox\_A(3)  
[#8](-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#6]:3:[#6]:[#6]:2:[#7]:o:[#7]:[#6]:2:[#6]:[#6]:3  
diazox\_B(3)  
[Cl]-[#6]:2:[#6]:[#6]:1:n:o:n:[#6]:1:[#6]:[#6]:2  
diazox\_C(1)  
[#7]-2=[#7]-[#6]:1:[#7]:[!#6&!#1]:[#7]:[#6]:1-[#7]=[#7]-[#6]:[#6]-2  
diazox\_D(1)  
[#6]-2(-[#1])(-[#8]-[#1])-[#6]:1:[#7]:[!#6&!#1]:[#7]:[#6]:1-[#6](-[#1])(-[#8]-[#1])-[#6]=[#6]-2  
diazox\_E(1)  
[#7](-[#1])(-[#1])-[#6]:1:[#6](-[#7](-[#1])-[#1]):[#6](:[#6](-[#1]):[#6]:2:[#7]:o:[#7]:[#6]:1:2)-[#1])  
diazox\_sulfon\_B(5)

[#6]:1:[#6](:[#6]:[#6]:[#6]:[#6]:1)-[#7]-2-[#6](-[#1])-[#6](-[#1])-[#7](-[#6](-[#1])-[#6]-2-[#1])-[#16](=[#8])(=[#8])-[#6]:3:[#6]:[#6]:[#6]:[#6]:4:[#7]:s:[#7]:[#6]:3:4  
dyes7A(2)  
[#6]:1:[#6](:[#6]:[#6]:[#6]:[#6]:1)-[#7](-[#6](-[#1])-[#1])-[#6](-[#1])=[#6](-[#1])-[#6](!@[#6](-[#1])-[#6](-[#1])=[#6]-[#6]@[#7]-[#6]:2:[#6]:[#6]:[#6]:[#6]:[#6]:2  
ene\_cyano\_B(7)  
[#6]-1(=[#6]-[#6](-[#6]:2:[#6]:[#6](:[#6](:[#7]:[#6]-1:2)-[#7](-[#1])-[#1])-[#6]#[#7])=[#6]-[#6]#[#7])  
ene\_cyano\_C(6)  
[#6]=[#6](-[#6]#[#7])-[#6]([#7]-[#1])-[#7]-[#7]  
ene\_cyano\_D(3)  
[#6](-[#6]#[#7])(-[#6]#[#7])=[#6](-[#16])-[#16]  
ene\_cyano\_E(1)  
[#8]=[#6]-[#6](-[#1])=[#6](-[#6]#[#7])-[#6]  
ene\_cyano\_F(1)  
[#8](-[#1])-[#6]([#8])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#8]-[#1])-[#1])-[#6]:2:[#6](-[#1]):[#6](:[#6](:o:2)-[#6](-[#1])=[#6](-[#6]#[#7])-[#6]:3:[#7]:[#6]:[#6]:[#7]:3)-[#1])-[#1])-[#1]  
ene\_cyano\_G(1)  
[#7]1(-[#6])[#6]([#6](-[#1])[#6]([#6]1-[#6](-[#1])=[#6](-[#6]#[#7])-[#6]:2:[#7]:[#6]:[#6]:s:2)-[#1])-[#1]  
ene\_five\_het\_G(10)  
[#6]-1(=[#8])-[#6]([#6](-[#1])-[#6]([#6]:1:[#6]:[#6]:[#6]:[#6]:1),\$([#6]:1:[#6]:[#6]:[#6]:[#6]:[#6]!#1:1))-  
[#7]=[#6](-[#1]:[#1]:[#1]:[#1])-[#6]([#16]),\$([#7]-[#1]:[#1])-1  
ene\_five\_het\_H(6)  
[#7]-1=[#6]-[#6](-[#6](-[#7]-1)=[#16])=[#6]  
ene\_five\_het\_I(6)  
[#6]:1:[#6]:[#6]:[#6]:o:1)-[#6](-[#1])=!@[#6]-3-[#6]([#8])-[#6]:2:[#6]:[#6]:[#6]:[#6]:[#6]:2-[#6&!#1]-3  
ene\_five\_het\_J(4)  
[#16]=[#6]-1-[#7](-[#1])-[#6]=[#6]-[#6]-2=[#6]-1-[#6]([#8])-[#8]-[#6]-2=[#6]-[#1]  
ene\_five\_het\_K(4)  
[#7]1(-[#6])[#6]([#6](-[#1])[#6]([#6]1-[#6](-[#1])=[#6]-2-[#6]([#8])-[#6]!#1-[#6]=,:[#1]-2)-[#1])-[#1]  
ene\_five\_het\_L(4)  
[#8]=[#6]-3-[#6](!@[#6](-[#1])-[#6]:1:[#6]:[#7]:[#6]:[#6]:1)-[#6]:2:[#6]:[#6]:[#6]:[#6]:[#6]:2-[#7]-3  
ene\_five\_het\_M(3)  
[#6]-1=,:[#6]-[#6](-[#6](-[#6](-[#6]([#8]),\$([#16])-1)=[#6]-[#6]([#8])=[#8]  
ene\_five\_het\_N(1)  
[#6]-2(=[#8])-[#6]([#6](-[#1])-[#6]:1:[#6](:[#6]:[#6]:[#6](:[#6]:1)-[F,C1,Br,I])-[#8]-[#6](-[#1])-[#1])-[#7]=[#6](-[#16]-[#6](-[#1])-[#1])-[#16]-2  
ene\_five\_one\_B(1)  
[#6]:2:[#6]:1-[#6](-[#6](-[#6](-[#6]:1:[#6](:[#6](:[#6]:2-[#1])-[#1])-[#1])-[#1])-[#1])=[#8])=[#6](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#1]  
ene\_misc\_A(5)  
[#6]-1=[#6]-[#6](-[#8]-[#6]-1-[#8])(-[#8])-[#6]  
ene\_misc\_B(2)  
[#6]:[#6]-[#6](-[#1])(-[#1])-[#6](-[#1])-[#6]([#8])-[#7]-2-[#6]([#8])-[#6]-1(-[#1])-[#6](-[#1])(-[#1])-[#6]([#8])-[#6](-[#1])(-[#1])-[#6]-1(-[#1])-[#6]-2=[#8]  
ene\_misc\_C(1)  
[#6]:1:[#6]:[#6]-2:[#6](:[#6]:[#6]:1)-[#6]=[#6]-[#6](-[#7]-2-[#6]([#8])-[#7](-[#1])-[#6]:3:[#6]:[#6](:[#6](:[#6]:[#6]:3)-[#8]-[#6](-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#6](-[#1])-[#1]  
ene\_misc\_D(1)  
[#6]:1-2:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#8]-[#6](-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#1])-[#6]([#6](-[#6])-[#16]-[#6]-2(-[#1])-[#1])-[#6]  
ene\_misc\_E(1)  
[#6]:1:[#6](:[#6]-2:[#6](:[#6](:[#6]:1-[#8]-[#6](-[#1])-[#1])-[#1])-[#6]=[#6]-[#6](-[#1])-[#16]-2)-[#1])-[#8]-[#6](-[#1])-[#1]  
ene\_one\_A(3)  
[!#1]:1:[!#1]:[!#1]:[!#1]([!#1]:[!#1]:1)-[#6](-[#1])=[#6](-[#1])-[#6](-[#7]-[#6]:2:[#6]:[#6]:3:[#6](:[#6]:2):[#6]:[#6]:[#6](:[#7]:3)-[#7](-[#6])-[#6])=[#8]  
ene\_one\_B(2)  
[#6](-[#16])(-[#7])=[#6](-[#1])-[#6]=[#6](-[#1])-[#6]=[#8]  
ene\_one\_C(1)  
[#6]-1(=[#8])-[#6](-[#6](-[#6]#[#7])=[#6](-[#1])-[#7])-[#6](-[#7])-[#6]=[#6]-1  
ene\_one\_D(1)  
[#6](-[#8]-[#1]):[#6]-[#6]([#8])-[#6](-[#1])=[#6](-[#6])-[#6]  
ene\_one\_amide\_A(1)  
[#6]:1:[#6](:[#6]:[#6]:[#6]:[#6]:1)-[#6](-[#1])-[#7]-[#6]([#8])-[#6](-[#7](-[#1])-[#6](-[#1])-[#1])=[#6](-[#1])-[#6]([#8])-[#6]:2:[#6]:[#6]:[#6](:[#6]:[#6]:2)-[#8]-[#6](-[#1])-[#1]  
ene\_one\_amide\_B(1)  
[#6]2-3:[#6]:[#6]:[#6]:1:[#6]:[#6]:[#6]:[#6]:1:[#6]2-[#6](-[#1])-[#6;X4]-[#7]-[#6]-3=[#6](-[#1])-[#6]([#8])-[#6](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1]  
ene\_one\_one\_A(1)  
[#8]=[#6]-[#6]-1=[#6](-[#16]-[#6]([#6](-[#1])-[#6])-[#16]-1)-[#6]=[#8]  
ene\_one\_one\_B(1)  
[#6]-1(-[#6]([#8])-[#6](-[#1])(-[#1])-[#6]-[#6](-[#1])(-[#1])-[#6]-1=[#8])=[#6](-[#7]-[#1])-[#6]=[#8]  
ene\_one\_yne\_A(1)  
[#6]#[#6]-[#6]([#8])-[#6]#[#6]  
ene\_quin\_methide(10)  
[!#1]:[!#1]-[#6](-[#6]([#6]#[#7]))=[#6]-1-[#6]=,:[#6]-[#6]([#6]([#8]),\$([#7;!R]))-[#6]=,:[#6]-1  
ene\_rhod\_C(13)

[#16]-1-[#6](=[#7]-[#6]:[#6])-[#7](-[extract\_itex]([#1]),[/extract\_itex]([#6](-[#1])(-[#1])-[#6](-[#1])(-[#1])-[#8]),[extract\_itex]([#6]:[#6])))-[#6](=[#8])-[#6]-1=[#6](-[#1])-[extract\_itex]([#6]:[#6]:[#6]-[#17]),[/extract\_itex]([#6]:[#6&!#1]))  
ene\_rhod\_D(8)  
[#16]-1-[#6](=[#7]-[#6]:[#6])-[#7](-[extract\_itex]([#1]),[/extract\_itex]([#7](-[#1])-[#6]:[#6]))-[#7](-[extract\_itex]([#1]),[/extract\_itex]([#6]:[#7]:[#6]:[#6]:[#16])))-[#6](=[#8])-[#6]-1=[#6](-[#1])-[#6]:[#6]-[extract\_itex]([#17]),[/extract\_itex]([#8]-[#6]-[#1]))  
ene\_rhod\_E(8)  
[#16]-1-[#6](=[#8])-[#7]-[#6](=[#16])-[#6]-1=[#6](-[#1])-[#6]:[#6]  
ene\_rhod\_F(8)  
[#7]:1:[#6]:[#6]:[#6]:[#6]:[#6]:1-[#6](-[#1])-[#1]-[#6](-[#1])=[#6]-2-[#6](=[#8])-[#7]-[#6](=[#6&!#1])-[#7]-2  
ene\_rhod\_G(7)  
[#8](-[#1])-[#6](=[#8])-[#6]:1:[#6]:[#6]:[#6]:[#6]:1-[#6]:[#6]:[#6](-[#1])=[#6]-2-  
[#6](=[#6&!#1])-[#7]-[#6](=[#6&!#1])-[#6&!#1]-2  
ene\_rhod\_H(5)  
[#7]-1-2-[#6](=[#7]-[#6](=[#8])-[#6](=[#7]-1)-[#6](-[#1])-[#1])-[#16]-[#6](=[#6](-[#1])-[#6]:[#6])-[#6]-  
2=[#8]  
ene\_rhod\_I(3)  
[#7]-2(-[#6](-[#1])-[#1])-[#6](=[#16])-[#7](-[#1])-[#6](=[#6](-[#1])-[#6]:1:[#6]:[#6]:[#6]:[#6]:[#6]:1)-  
[Br])-[#6]-2=[#8]  
ene\_rhod\_J(3)  
[#6](-[#1])(-[#1])-[#7]-2-[#6](=[extract\_itex]([#16]),[/extract\_itex]([#7]))-[#6&!#1]-[#6](=[#6]-1-[#6](=[#6](-[#1])-[#6]:[#6]-[#7]-  
1-[#6](-[#1])-[#1])-[#1])-[#6]-2=[#8]  
ene\_rhod\_J\_bis(3)  
[#6][#7]1[#6](=[extract\_itex]([#16]),[/extract\_itex]([#7]))[!#6&!#1][#6](=c2[cH1][cH1]ccn2[#6H2])[#6]1=[#8]  
ene\_six\_het\_B(2)  
[#6]:1:[#6]:[#6]:[#6]:[#6]:1-[#6](=[#8])-[#6](-[#1])=[#6]-3-[#6](=[#8])-[#7](-[#1])-[#6](=[#8])-  
[#6](=[#6](-[#1])-[#6]:2:[#6]:[#6]:[#6]:[#6]:[#6]:2)-[#7]-3-[#1]  
ene\_six\_het\_C(2)  
[#8]=[#6]-1-[#6]:[#6]-[#6](-[#1])(-[#1])-[#7]-[#6]-1=[#6]-[#1]  
ene\_six\_het\_D(1)  
[#8]=[#6]-1-[#7]-[#7]-[#6](=[#7]-[#6]-1=[#6]-[#1])-[!#1]:[#1]  
furan\_A(3)  
[#6]:1:[#6]:[#6]:[#6]:1-[#6](-[#1])-[#1])-[#1])-[#1])-[#6](-[#1])(-[#8]-[#1])-[#6]#[#6]-[#6;X4]  
furan\_acid\_A(4)  
[#6]:1:[#6]:[#6]:[#6]:1-[#6](-[#1])-[#1])-[#6](-[#1])(-[#1])-[#8]-[#6]:[#6]-[#1])-[#6](=[#8])-[extract\_itex]([#8-  
1]),[/extract\_itex]([#8]-[#1]))  
het\_465\_misc(1)  
[#6]:1-2:[#6]:[#6]-3:[#6]:[#6]:1-[#8]-[#6]-[#8]-2-[#6]-[#6]-3  
het\_55\_A(2)  
[#6]:[#6]-[#7]:2:[#7]:[#6]:1-[#6](-[#1])(-[#1])-[#16;X2]-[#6](-[#1])(-[#1])-[#6]:1-[#6]:2-[#7](-[#1])-  
[#6](=[#8])-[#6](-[#1])=[#6]-[#1]  
het\_55\_B(1)  
[#6]-1:[#6]-[#8]-[#6]-2-[#6](-[#1])(-[#1])-[#6](=[#8])-[#8]-[#6]-1-2  
het\_565\_A(2)  
[#6]:1:2:[#6]:3:[#6]:[#6](-[#8]-[#1]):[#6]:[#6]:1:[#6]:[#6]:[#7]:2-[#6]-[#6]=[#8]-[#1]:[#7]:[#6]:[#7]:3  
het\_565\_indole(1)  
[#6]2([#6](-[#1])[#7](-[#6](-[#1])-[#1])[#6]:3:[#6]:[#6]:1:[#7]([#6]([#6]([#6]:1:[#6]2:3)-[#1])-[#1])-  
[#6](-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#1]  
het\_5\_A(7)  
[#7]-2(-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#7]=[#6](-[#6]=[#8])-[#6;X4]-[#6]-2=[#8]  
het\_5\_B(4)  
[#7]-2(-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#7]=[#6](-[#7](-[#1])-[#6]=[#8])-[#6](-[#1])(-[#1])-[#6]-2=[#8]  
het\_5\_C(2)  
[#7]-2=[#6](-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#6](-[#1])(-[#1])-[#6](-[#8]-[#1])(-[#6](-[#9])(-[#9])-  
[#9])-[#7]-2-[extract\_itex]([#6]:[#6]:[#6]:[#6]:[#6]:[#6]),[/extract\_itex]([#6](-[#16])-[#6]:[#6]:[#6]:[#6]:[#6]:[#6]))  
het\_5\_D(2)  
[#7]-2(-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#7]=[#6](-[#6](-[#1])-[#1])-[#6](-[#1])(-[#16]-[#6])-[#6]-2=[#8]  
het\_5\_E(1)  
[#7]-3(-[#6]:2:[#6]:1:[#6]:[#6]:[#6]:[#6]:1:[#6]:[#6]:[#6]:2)-[#7]=[#6](-[#6](-[#1])-[#1])-[#6](-[#1])(-  
[#1])-[#6]-3=[#8]  
het\_5\_ene(1)  
[#6]-2(=[#8])-[#6](=[#6](-[#6](-[#1])-[#1])-[#7](-[#1])-[#6](-[#1])(-[#1])-[#6](-[#1])(-[#1])-[#6](-[#1])-  
[#1])-[#7]=[#6](-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#8]-2  
het\_5\_inium(1)  
[#7]-4(-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#6](=[#7+])(-[#6]:2:[#6]:[#6]:[#6]:[#6]:2)-[#6](=[#7]-  
[#6]:3:[#6]:[#6]:[#6]:[#6]:3)-[#7]-4)-[#1]  
het\_5\_pyrazole\_OH(14)  
[#6]1([#7][#7]([#6]([#6]1-[extract\_itex]([#1]),[/extract\_itex]([#6]-[#1]))-[#8](-[#1])-[#6]:2:[#6]:[#6]:[#6]:2-[#1])-  
[#1])-[#1])-[#1])-[#6;X4]  
het\_65\_B(7)  
[!#1]:1:[!#1]-2:[!#1]([!#1]:[!#1]:[!#1]:1)-[#7](-[#1])-[#7](-[#6]-2=[#8])-[#6]  
het\_65\_B\_bis(7)  
[!#1]:1:[!#1]-,2:[!#1]([!#1]:[!#1]:[!#1]:1)-,:[#7](-[#1])-,:[#7](-,:[#6]-,2=[#8])-[#6]  
het\_65\_C(6)  
[#7]2[#6]1[#6][#6][#6][#6][#6]1[#6]([#6]2-[extract\_itex]([#6](-[#1])=[#6](-[#1])-[#6]:[#6]),[/extract\_itex]([#6]:[#8]:[#6]))-[#7]-  
[#6]:[#6]  
het\_65\_Da(2)  
[#7]2[#7][#6]([#6]1[#6][#6][#6]1[#6]2-[#6])-[#6]  
het\_65\_Db(5)  
[#6]3[#6][#7]1[#6]([#7][#6]([#6]1-[#7]-[#6])-[#6]:2:[#6]:[#6]:[#6]:[#6]:[#7]:2)[#6][#6]3

het\_65\_E(2)  
s1[#6]([#6]([#6]-2[#6]1-[#7](-[#1])-[#6](-[#6](=[#6]-2-[#1])-[#6]([#8])-[#6]([#8-1]),\$([#8]-[#1]))=[#8])-[#7](-[#1])-[#1])-[#6]([#8])-[#7]-[#1])  
het\_65\_F(1)  
s2[#6]:1:[#7]:[#6]:[#7]:[#6]([#6]:1[#6]([#6]2-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#7]-[#7]=[#6]-[#6]3[#6]3[#6]3o3  
het\_65\_G(1)  
[#6]-2(=[#7]-[#6]1[#6]([#6]([#7][#7]1-[#6](-[#6]-2(-[#1])-[#1])=[#8])-[#7](-[#1])-[#1])-[#7](-[#1])-[#1])-[#6])  
het\_65\_H(1)  
[#6]2([#6]-1[#7](-[#6](-[#6]=[#6]-[#7]-1)=[#8])[#7][#6]2-[#6]3[#6][#6][#6][#7]3)-[#6]#[#7]  
het\_65\_I(1)  
[#7]:1:2:[#6]:[#6]:[#6]([#6]:[#6]:1:[#6]:[#6]([#6]:2-[#6]([#8])-[#6]:[#6])-[#6]:[#6](-[#6]~[#8])~[#8])  
het\_65\_J(1)  
o:1:[#6]([#6]:[#6]:2:[#6]:1:[#6]([#6]([#6]([#6]([#6]:2-[#1])-[#8]-[#6](-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#1])-[#6]([#6]~[#8])~[#8])  
het\_65\_K(1)  
[#7]1[#7][#7][#6]2[#6][#6][#6][#6]12  
het\_65\_L(1)  
[#6]:1-2:[#6](-[#1]):s:[#6]([#6]:1-[#6]([#8])-[#7]-[#7]=[#6]-2-[#7](-[#1])-[#1])-[#6]=[#8])  
het\_65\_imidazole(1)  
[#6]2([#7][#6]:1:[#6]([#6]([#6]([#6]([#6]:1-[#1])-[#1])-[#1])-[#1])[#7]2-[#6]-[#7](-[#1])-[#6](-[#7](-[#1])-[#6]:3:[#6]([#6]:[#6]:[#6]:[#6]:3-[#1])-[#1])=[#8])  
het\_65\_mannich(1)  
[#6]:1-2:[#6]([#6]([#6]([#6]([#6]:1-[#8]-[#6](-[#1])-[#1])-[#8]-2-[#6](-[#1])-[#1])-[#7]-3-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#6]:[#6]-3-[#1])-[#1])-[#1])  
het\_65\_pyridone\_A(3)  
[#6]:2([#6](-[#6](-[#1])-[#1]):[#6]-1:[#6](-[#7]=[#6](-[#7](-[#6]-1=[#6&!#1;X1])-[#6](-[#1])-[#6]([#6]([#8])-[#8]),\$([#6]:[#6]))-[\$([#1]),\$([#16]-[#6](-[#1])-[#1]))]:[!#6&!#1;X2]:2)-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])  
het\_6666\_A(2)  
[#6]:2:[#6]:[#6]:1:[#7]:[#6]:3:[#6]([#7]:[#6]:1:[#6]:[#6]:2):[#6]:[#6]:[#6]:4:[#6]:3:[#6]:[#6]:[#6]:[#6]:4  
het\_666\_A(5)  
[#7]-2-[#6]:1:[#6]:[#6]:[#6]:[#6]:[#6]:1-[#6]([#7])-[#6]:3:[#6]-2:[#6]:[#6]:[#6]:[#6]:3  
het\_666\_A\_bis(5)  
[#7]-,2-,:[#6]:1:[#6]:[#6]:[#6]:[#6]:[#6]:1-,:[#6]([#7]),-,:[#6]:3:[#6]-,2:[#6]:[#6]:[#6]:[#6]:3  
het\_666\_B(3)  
[#6]:1:[#6]-3:[#6]([#6]:[#6]:[#6]:1)-[#7](-[#6]:2:[#6]:[#6]:[#6]:[#6]:2-[#8]-3)-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])  
het\_666\_C(1)  
[#6]:2-3:[#6]([#6]:[#6]:1:[#6]:[#6]:[#6]:[#6]:1:[#6]:2)-[#7](-[#6](-[#1])-[#1])-[#6]([#8])-[#6]([#7]-3)-[#6]:[#6]-[#7](-[#1])-[#6](-[#1])-[#1])  
het\_66\_A(7)  
[#6]:2:[#6]:[#6]:1:[#7]:[#7]:[#6]([#7]:[#6]:1:[#6]:[#6]:2)-[#6](-[#1])-[#1])-[#6]=[#8]  
het\_66\_B(2)  
[#6]:1:[#6]:[#6]:2:[#6]([#6]:1):[#7]:[#6]([#7]:[#6]:2)-[#7](-[#1])-[#6]-3=[#7]-[#6](-[#6]=[#6]-[#7]-3)-[#1])-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])  
het\_66\_C(2)  
[#6]:1:2:[#7]:[#6]([#6]([#7]:[#6]:1:[#6]:[#6]:[#6]:[1#1]:2)-[#6](-[#1])=[#6](-[#8]-[#1])-[#6]-[#6](-[#1])=[#6](-[#8]-[#1])-[#6])  
het\_66\_D(1)  
[#6]:2:[#6]:[#6]:1:[#7]:[#6]([#6]([#7]:[#6]:1:[#6]:[#6]:2)-[#6](-[#1])-[#1])-[#6]([#8])-[#6]:[#6]-[#6](-[#1])-[#1])-[#6]([#8])-[#6]:[#6])  
het\_66\_E(1)  
[#6]:2:[#6]:[#6]:1:[#7]:[#6]([#6]([#7]:[#6]:1:[#6]:[#6]:2)-[#6]:3:[#6]:[#6]:[#6]:[#6]:3)-[#6]:4:[#6]:[#6]:[#6]:[#6]:4-[#8]-[#1])  
het\_66\_anisole(1)  
[#6](-[#1])-[#1])-[#8]-[#6]:1:[#6]([#6]([#6]([#6]([#6]([#6]:1-[#1])-[#1])-[#1])-[#1])-[#7](-[#1])-[#6]([#6]([#6]:[#6]:[#6]:[#6]:3-[#8]-[#6](-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])  
het\_6\_hydroxyridone(1)  
[#7]-1=[#6](-[#7](-[#6](-[#6](-[#6]-1(-[#1])-[#6]:[#6])-[#1])-[#1])=[#8])-[#1])-[#7]-[#1])  
het\_6\_imidate\_A(4)  
[#7]=[#6]-1-[#7](-[#1])-[#6]([#6](-[#7]-[#1])-[#7]=[#7]-1)-[#7]-[#1])  
het\_6\_imidate\_B(1)  
[#7](-[#1])-[#6]:1:[#6]([#6]([#6]([#6]([#6]:1-[#1])-[#1])-[#1])-[#1])-[#8]-[#1])-[#6]-2=[#6](-[#8]-[#6](-[#7]=[#7]-2)-[#7](-[#1])-[#1])  
het\_6\_pyridone\_NH2(1)  
[#8](-[#1])-[#6]:1:[#6]([#6]:[!#1]:[#6]([#7]:1)-[#7](-[#1])-[#1])-[#6](-[#1])-[#1])-[#6]([#8])-[#8])  
het\_6\_pyridone\_OH(5)  
[#8](-[#1])-[#6]:1:[#7]:[#6]([#6]:[#6]:[#6]:1)-[#8]-[#1])  
het\_76\_A(1)  
s:1:[#6]([#6](-[#1]):[#6]([#6]:1-[#6]-3=[#7]-[#6]:2:[#6]:[#6]:[#6]:[#6]:2-[#6]([#7]-[#7]-3-[#1])-[#6]:4:[#6]:[#6]:[#7]:[#6]:[#6]:4)-[#1])-[#1])  
het\_pyraz\_misc(1)  
[#6](-[F])-[F]-[#6]([#8])-[#7](-[#1])-[#6]:1:[#6](-[#1]):[#7](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#6]:[#6]:[#7]:[#6]:1-[#1])  
het\_pyridiniums\_B(2)  
[#6]:1:2:[!#1]:[#7+]:[#6]([!#1]:1:[#6]:[#6]:[#6]:[#6]:2)-[\*]~[#6]:[#6])  
het\_pyridiniums\_C(1)

[#6]~1~3~[#7](-[#6]:[#6])~[#6]~[#6]~[#6]~[#6]~1~[#6]~2~[#7]~[#6]~[#6]~[#6]~[#6]~[#7+]~2~[#7]~3  
het\_thio\_5\_A(8)  
[#6](-[#1])(-[#1])-[#16;X2]-[#6]:1:[#7]:[#6](:[#6](:[#7]:1-!@[#6](-[#1])-[#1])-  
[#6]:2:[#6]:[#6]:[#6]:[#6]:2)-[#1]  
het\_thio\_5\_B(2)  
[#6]-1(-[#6]=[#8])(-[#6]:[#6])-[#16;X2]-[#6]=[#7]-[#7]-1-[#1]  
het\_thio\_5\_C(2)  
[#16]=[#6]-2-[#7](-[#1])-[#7]=[#6](-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-  
[#1])-[#1])-[#8]-2  
het\_thio\_5\_C\_bis(2)  
[#16]=c2[nH]nc(c1[cH][cH]c([cH][cH]1)[#8][#6]([#1])([#1]))o2  
het\_thio\_5\_imine\_A(1)  
[#7]=[#6]-1-[#16]-[#6](=[#7])-[#7]=[#6]-1  
het\_thio\_5\_imine\_B(1)  
[#7]-1(-[#6](-[#1])-[#1])-[#6](=[#16])-[#7](-[#6]:[#6])-[#6](=[#7]-[#6]:[#6])-[#6]-1=[#7]-[#6]:[#6]  
het\_thio\_5\_imine\_C(1)  
[#16]-1-[#6](=[#7]-[#7]-[#1])-[#16]-[#6](=[#7]-[#6]:[#6])-[#6]-1=[#7]-[#6]:[#6]  
het\_thio\_656a(5)  
[#6]:1:3:[#6](:[#6]:[#6]:[#6]:[#6]:1):[#6]:2:[#7]:[#7]:[#6](-[#16]-[#6](-[#1])-[#1])-  
[#6]=[#8]:[#7]:[#6]:2:[#7]:3-[#6](-[#1])-[#1]-[#6](-[#1])=[#6](-[#1])-[#1]  
het\_thio\_656b(3)  
[#6]-[#6](=[#8])-[#6](-[#1])-[#1]-[#16;X2]-  
[#6]:3:[#7]:[#7]:[#6]:2:[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1:[#7](:[#6]:2:[#7]:3)-[#1])-[#1])-[#1])-[#1])-  
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het\_thio\_656c(1)  
[#6]:1:[#6](:[#6]:[#6]:[#6]:[#6]:1)-[#6]-4=[#7]-[#7]:2:[#6](:[#7+]:[#6]:3:[#6]:2:[#6]:[#6]:[#6]:[#6]:3)-  
[#16]-[#6;X4]-4  
het\_thio\_65\_A(3)  
[#6](-[#1])(-[#1])-[#16;X2]-[#6]3[#7][#6]1[#6]([#7]([#7][#6]1-[#6](-[#1])-[#1])-  
[#6]:2:[#6]:[#6]:[#6]:[#6]:2)[#7][#7]3  
het\_thio\_65\_B(2)  
[#7](-[#1])-[#6]1[#7][#6]([#7][#6]2[#7][#7][#6]([#7]12)-[#16]-[#6])-[#7](-[#1])-[#6]  
het\_thio\_65\_C(2)  
[#7]:1:[#6](:[#7](:[#6]:2:[#6]:1:[#6]:[#6]:[#6]:[#6]:2)-[#6](-[#1])-[#1]-[#16]-[#6](-[#1])-[#1])-  
[#6](=[#8])-[#7](-[#1])-[#7]=[#6](-[#1])-[#6](-[#1])=[#6]-[#1]  
het\_thio\_65\_D(1)  
[#6]:2(:[#7]:[#6]:1:[#6](:[#6](:[#6]:[#6](:[#6]:1-[#1])-[F,C1,Br,I]-[#1]):[#7]:2-[#1])-[#16]-[#6](-[#1])-  
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het\_thio\_665(1)  
[#6]:1:[#6]:[#6]-2:[#6](:[#6]:[#6]:1)-[#16]-[#6]3[#6](-[#7]-2)[#6][#6](s3)-[#6](-[#1])-[#1]  
het\_thio\_666\_A(13)  
[#6]:2(:[#6]:1-[#16]-[#6]:3:[#6](-[#7](-[#6]:1:[#6](:[#6](:[#6]:2-[#1])-[#1])-[#1])-[#6](-[#1])-  
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\$([#1]),\$([#7](-[#1])-[#1]),\$([#8]-[#6;X4]))~\$([#1]),\$([#7](-[#1])-[#6;X4]),\$([#6]:[#6]))-[#1]  
het\_thio\_66\_A(3)  
[#6]:1-2:[#6](:[#6]:[#6]:[#6]:[#6]:1)-[#6](-[#1])-[#1]-[#6](-[#1])-[#1]-[#7]=[#6]-2-[#16;X2]-[#6](-  
[#1])-[#1]-[#6](=[#8])-[#6]:3:[#6]:[#6]:[#6]:[#6]:3  
het\_thio\_66\_one(8)  
[#6](=[#8])-[#6]-1=[#6]-[#7]-[#6]:2:[#6](-[#16]-1):[#6]:[#6]:[#6]:[#6]:2  
het\_thio\_676\_A(10)  
[#6]:1:[#6]:[#6]-2:[#6](:[#6]:[#6]:1)-[#6]-[#6](-[#6]:3:[#6](-[#16]-2):[#6](:[#6](-[#1]):[#6](:[#6]:3-[#1])-  
\$([#1]),\$([#8]),\$([#16;X2]),\$([#6;X4]),\$([#7](-\$([#1]),\$([#6;X4]))-[\$([#1]),\$([#6;X4]))])-[#1])-[#7](-  
\$([#1]),\$([#6;X4]))-[\$([#1]),\$([#6;X4]))]  
het\_thio\_676\_B(1)  
[#6]:1-2:[#6](:[#6](:[#6](:[#6]:1-[#6](-[#6]:3:[#6](-[#16]-[#6]-2(-[#1])-[#1]):[#6](:[#6](-  
[#1]):[#6](:[#6]:3-[#1])-[#1])-[#1])-[#8]-[#6]:[#6]-[#1])-[#1])-[#1])-[#1]  
het\_thio\_67\_A(1)  
[#6](-[#1])(-[#1])-[#16;X2]-[#6]:2:[#7]:[#7]:[#6]:1-[#6]:[#6]-[#7]=[#6]-[#8]-[#6]:1:[#7]:2  
het\_thio\_6\_ene(2)  
[#6]-1:[#6]-[#7]=[#6]-[#6](=[#6]-[#7]-[#6])-[#16]-1  
het\_thio\_6\_furan(4)  
[#6](-[#1])(-[#1])-[#16;X2]-[#6]:1:[#7]:[#7]:[#6](:[#6](:[#7]:1)-[#6]:2:[#6](:[#6](:[#6](:o:2)-[#1])-[#1])-  
[#1])-[#6]:3:[#6](:[#6](:[#6](:o:3)-[#1])-[#1])-[#1]  
het\_thio\_N\_55(5)  
[#6](-[#1])-[#6]:2:[#7]:[#7](-[#6]:1:[#6]:[#6]:[#6]:[#6]:1):[#16]:3:[!#6&!#1]:[!#1]:[#6]:[#6]:2:3  
het\_thio\_N\_5A(3)  
[#7]=[#6]-1-[#7]=[#6]-[#7]-[#16]-1  
het\_thio\_N\_5A\_bis(3)  
n1cnc(=[#7])s1  
het\_thio\_N\_5B(2)  
[#6]~1~[#6](-[#7]~[#7]~[#6](-[#6](-[#1])-[#1])~[#6](-[#1])-[#1])~[#7]~[#16]-[#6]~1  
het\_thio\_N\_5C(1)  
[#6]:[#6]-[#7](-[#1])-[#6](=[#8])-[#6]1[#6](s[#7][#7]1)-[#7](-[#1])-[#6]:[#6]  
het\_thio\_N\_5D(1)  
[#7]1[#7]s[#6][#6]1-[#6]2[#7][#6]([#7]o2)-[#6]:[#6]  
het\_thio\_N\_65A(3)  
[#7]-2-[#16]-[#6]-1=[#6](-[#6]:[#6]-[#7]-[#6]-1)-[#6]-2=[#16]  
het\_thio\_pyr\_A(3)

[#7]:1:[#6](:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#16]-[#6]-[#1])-[#6]#[#7])-[#6]:2:[#6]:[#6]:[#6](:[#6]:[#6]:2)-[#8]-[#6](-[#1])-[#1]-[#1])-[#6]:[#6] )  
het\_thio\_urea\_ene(1)  
[#6]-1(=[#7]-[#7](-[#6](-[#16]-1)=[#6](-[#1])-[#6]:[#6])-[#6]:[#6])-[#6]=[#8]  
hydroquin\_A(2)  
[#6]:1(:[#6]:[#6](:[#6](:[#6]:[#6]:1)-[#8]-[#1])-[#6](=[#6]-[#7])-[#6]=[#8])-[#8]-[#1]  
hzide\_naphth(2)  
[#6]:2(:[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1:[#6](:[#6](:[#6]:2-[#1])-[#1])-[#1])-[#1])-[#7](-[#1])-[#7](-[#1])-[#6]=[#8])-[#1]-[#1])-[#1])-[#1]  
hzone\_acid\_A(1)  
[#6]:1-3:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#6]([#7]-[#7](-[#1])-[#6]:2:[#6](:[#6](:[#6](:[#6](:[#6]:2-[#1])-[#1])-[#6]([#8])-[#8]-1),#[#8]-[#1]))-[#1]-[#1])-[#6]:4:[#6]-3:[#6](:[#6](:[#6](:[#6]:4-[#1])-[#8]-[#6](-[#1])-[#1])-[#1])-[#1])-[#1]  
hzone\_acid\_D(1)  
[#8](-[#1])-[#6]([#8])-[#6]:1:[#6]:[#6]:[#6](:[#6]:[#6]:1)-[#7]-[#7]=[#6](-[#1])-[#6]:2:[#6](:[#6](:[#6](:[#6](:[#6]:2)-[#6]:3:[#6]:[#6]:[#6]:[#6]:[#6]:3)-[#1])-[#1]  
hzone\_acyl\_misc\_A(1)  
[#6]:1(:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#6]([#8])-[#7](-[#1])-[#7]=[#6](-[#1])-[#6](:[#6](:[#6](:[#6](:[#6]:2-[\*]-[\*]-[\*]-[#6]:3:[#6]:[#6]:[#6]:o:3  
hzone\_acyl\_misc\_B(1)  
[#7]:1:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#1])-[#6]([#8])-[#7](-[#1])-[#7]=[#6](-[#1])-[#6]:2:[#6](:[#6](:[#6]:2-[#8]-[#6](-[#1])-[#1])-[#6]([#8])-[#8]-1),#[#8]-[#1]))  
hzone\_anil(14)  
[#6]:1(:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#7](-[#1])-[#1])-[#1])-[#6]([#7]-[#7]-[#1])  
hzone\_anthran\_Z(1)  
[#6]:1:[#6]:2:[#6](:[#6]:[#6]:[#6]:1):[#6](:[#6]:3:[#6](:[#6]:2):[#6]:[#6]:[#6]:[#6]:3)-[#6]([#7]-[#7](-[#1])-[#6]:4:[#6]:[#6]:[#6]:[#6]:4  
hzone\_furan\_A(6)  
[#6]:1(:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#6]([#8])-[#7](-[#1])-[#7]=[#6](-[#1])-[#6]:2:[#7]:[#6]:[#6]:s:2  
hzone\_furan\_B(2)  
[#6]:1(:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#6]([#8])-[#7](-[#1])-[#7]=[#6](-[#1])-[#6]:2:[#7]:[#6]:[#6]:s:2  
hzone\_furan\_C(1)  
[#6]:1:[#6](:[#6]:[#6]:[#6]:1)-[#7](-[#6]:2:[#6]:[#6]:[#6]:[#6]:2)-[#7]=[#6](-[#1])-[#6]:3:[#6](:[#6](:[#6](:[#6]:3)-[#6]:4:[#6]:[#6]:[#6](:[#6]:4)-[#6]([#8])-[#8]-1),#[#8]-[#1]))-[#1]-[#1]  
hzone\_furan\_E(1)  
[#8](-[#1])-[#6]([#8])-[#6]:1:[#6]:[#6]:[#6]:[#6](:[#6]:1)-[#6]:[#6]:[#6]([#7]-[#7](-[#1])-[#6]([#8])-[#6](-[#1])-[#1])-[#8]  
hzone\_naphth\_A(5)  
[#6]:1:2:[#6](:[#6](:[#6](:[#6](:[#6]:1:[#6](:[#6](:[#6](:[#6]:2-[#1])-[#1])-[#6]([#7]-[#7](-[#1])-[#6]([#6]:[#6]),#[#6]=[#16]))-[#1]-[#1])-[#1])-[#1])-[#1]  
hzone\_phenone(7)  
[#6](-[#6]:1:[#6](:[#6](:[#6](:[#6]:[#6]:1-[#1])-[#6]([#6;X4]),#[#1]))-[#1]-[#1])-[#6]:2:[#6](:[#6](:[#6](:[#6]:2-[#1])-[#1])-[#6]([#1]),#[#17]))-[#1]-[#1])-[#6]([#7]-[#8]-[#6](-[#1])-[#1])-[#6](-[#1])-[#6](-[#1])-[#6](-[#1])-[#7](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1]),#[#7]-[#8]-[#6](-[#1])-[#1])-[#6](-[#1])-[#6](-[#1])-[#7](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1]),#[#7]-[#7](-[#1])-[#6]([#7]-[#7](-[#1])-[#6]([#7]-[#7](-[#1])-[#6]([#6]&[#1]:[#6](:[#6]:2-[#6](-[#1])=[#7]-[#7](-[#1])-[#6]([#6]:1):[#6]([#6](-[#1]):[#16]:1),#[#6]:[#6](-[#1]):[#6]-[#1]),#[#6]:[#7]:[#6]:[#7]:[#6]:[#7]),#[#6]:[#7]:[#7]:[#7]:[#7]))-[#6]([#1]),#[#8]-[#1]),#[#6](-[#1])-[#1])  
hzone\_thiophene\_B(4)  
[#6]:1(:[#6](:[#6](:[#6](:s:1)-[#1])-[#1])-[#6]([#1]),#[#6](-[#1])-[#1]))-[#6](-[#1])=[#7]-[#7](-[#1])-[#6]:2:[#6]:[#6]:[#6]:[#6]:2  
imidazole\_B(2)  
[#6](-[#1])-[#6](-[#1])-[#1]-[#16]-[#6](-[#1])-[#1]-[#6]1[#6][#7]([#6][#7]1)-[#1]  
imidazole\_B\_bis(2)  
[#6](-[#1])-[#1][#6](-[#1])-[#1][#16][#6](-[#1])-[#1][#6]1[#6][#7][#6][#7]([#1])1  
imidazole\_C(1)  
[#6]-3(-[#1])-[#7]:1:[#6](:[#7]:[#6](:[#6]:1-[#1])-[#1])-[#6]:2:[#6](:[#6](:[#6](:[#6]:2-[#1])-[#6]([#6](-[#1])-[#1])-[#6](-[#1])-[#6](-[#1])-[#6](-[#1])-[#6]:4:[#6]-3:[#6](:[#6](:[#6](:[#6]:4-[#1])-[#1])-[#1])-[#1]  
imidazole\_amino\_A(1)  
[#7]:1:[#6](:[#7](:[#6](:[#6]:1-[#6]:2:[#6]:[#6]:[#6]:[#6]:2)-[#6]:3:[#6]:[#6]:[#6]:[#6]:3)-[#7]=!#[#6]-[#7](-[#1])-[#1]  
imine\_ene\_A(5)  
[#6]:[#6]-[#6](-[#1])=[#6](-[#1])-[#6](-[#1])=[#7]-[#7](-[#6;X4])-[#6;X4]  
imine\_ene\_one\_A(3)  
[#6]-2(-[#6]=[#7]-[#6]:1:[#6]:[#6]:[#6]:[#6]:1-[#7]-2)=[#6](-[#1])-[#6]=[#8]  
imine\_ene\_one\_B(1)  
[#6]-1:[#6]-[#6]([#8])-[#6]=[#6]-1-[#7]=[#6](-[#1])-[#7](-[#6;X4])-[#6;X4]  
imine\_imine\_A(9)  
[#6]:1:[#6]:[#6]-2:[#6](:[#6]:[#6]:1)-[#7]=[#6]-[#6]-2=[#7;!R]  
imine\_imine\_B(3)  
[#6]:[#6]-[#6](-[#1])=[#6](-[#1])-[#6](-[#1])=[#7]-[#7]=[#6]  
imine\_imine\_C(3)

[#7](-[#6](-[#1])-[#1])(-[#6](-[#1])-[#1])-[#6](-[#1])=[#7]-[#6](-[#6](-[#1])-[#1])=[#7]-[#7](-[#6](-[#1])-[#1])-[#6]:[#6]  
imine\_naphthol\_A(1)  
[#6]:1:2:[#6](:[#6](:[#6](:[#6](:[#6]:1:[#6](:[#6](:[#6](:[#6]:2-[#1])-[#1])-[#6]([#7]-[#6]:[#6])-[#6](-[#1])-[#1])-[#8]-[#1])-[#1])-[#1])-[#1])-[#1])-[#1]  
imine\_one\_B(4)  
[#7](-[#1])(-[#6]:1:[#6]:[#6]:[#6]:[#6]:[#6]:1)-[#7]=[#6](-[#6]([#8])-[#6](-[#1])-[#1])-[#7](-[#1])-[#6]([#7]-[#1]),\$([#6]:[#6])]  
imine\_one\_fives\_B(9)  
[#7;!R]=[#6]-2-[#6]([#8])-[#6]:1:[#6]:[#6]:[#6]:[#6]:[#6]:1-[#16]-2  
imine\_one\_fives\_C(2)  
[#6]:[#6]-[#7;!R]=[#6]-2-[#6]([#6&!#1])-[#6]:1:[#6]:[#6]:[#6]:[#6]:[#6]:1-[#7]-2  
imine\_one\_fives\_D(1)  
[#6]-1(=[#6&!#1])-[#6](-[#7]=[#6]-[#16]-1)=[#8]  
imine\_phenol\_A(3)  
[#6]=[#7;!R]-[#6]:1:[#6]:[#6]:[#6]:[#6]:[#6]:1-[#8]-[#1]  
indole\_3yl\_alk\_B(1)  
[#6]:12:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#1])-[#1])-[#1])-[#6]([#6](-[#6]:[#6])[#7]2-!@[#6]:[#6])-[#6](-[#1])-[#1]  
keto\_keto\_beta\_B(12)  
[#6;X4]-1-[#6]([#8])-[#7]-[#7]-[#6]-1=[#8]  
keto\_keto\_beta\_C(7)  
[#6]:1:[#6]:[#6]-2:[#6](:[#6]:[#6]:1)-[#6]([#6](-[#6]-2=[#8])-[#6])-[#8]-[#1]  
keto\_keto\_beta\_D(5)  
[#8]=[#6]-[#6]=[#6](-[#1])-[#8]-[#1]  
keto\_keto\_beta\_E(1)  
[#6]([#8])-[#6](-[#1])=[#6](-[#8]-[#1])-[#6](-[#8]-[#1])=[#6](-[#1])-[#6]([#8])-[#6]  
keto\_keto\_beta\_F(1)  
[#6](-[#1])(-[#1])-[#6](-[#8]-[#1])=[#6](-[#6]([#8])-[#6](-[#1])-[#1])-[#6](-[#1])-[#6]#[#6]  
keto\_keto\_beta\_zone(1)  
[#6]:[#6]-[#7](-[#1])-[#7]=[#6](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#6](-[#6](-[#1])-[#1])=[#7]-[#7](-[#1])-[#6]:[#6]  
keto\_keto\_gamma(5)  
[#8]=[#6]-1-[#6;X4]-[#6]-[#6]([#8])-[#6]:2:[#6]:[#6]:[#6]:[#6]:[#6]-1:2  
keto\_naphthol\_A(2)  
[#6]:1:2:[#6]:[#6]:[#6]:[#6](:[#6]:1:[#6](:[#6]:[#6]:[#6]:2)-\$([#8]-[#1]),\$([#7](-[#1])-[#1]))-[#6](-[#6])=[#8]  
keto\_phenone\_A(11)  
[#6]:1:[#6]-3:[#6](:[#6]:[#6]:[#6]:1)-[#6]:2:[#7]:[!#1]:[#6]:[#6]:[#6]:2-[#6]-3=[#8]  
keto\_phenone\_B(1)  
[#6]:1:[#6]-3:[#6](:[#6]:[#6]:[#6]:1)-[#6]-2=[#7]-[!#1]=[#6]-[#6]-[#6]-2-[#6]-3=[#8]  
keto\_phenone\_C(1)  
[#6]:2(:[#6]:1:[#6]:[#6]:[#6]:[#6]:1:[#6]-3:[#6](:[#6]:2)-[#6](-[#6]:4:[#6]:[#6]:[#6]:[#6]:[#6]-3:4)=[#8]-[#8]-[#1]  
keto\_phenone\_zone\_A(2)  
[#6]:1:[#6]:[#6]:[#6]:[#6]:[#6]:1-[#6]([#8])-[#7](-[#1])-[#7]=[#6]-3-[#6]:2:[#6]:[#6]:[#6]:[#6]:[#6]:2-[#6]:4:[#6]:[#6]:[#6]:[#6]-3:4  
keto\_thiophene(3)  
[#6]:1(:[#6](:[#6]:2:[#6](:s:1):[#6]:[#6]:[#6]:[#6]:2)-[#6](-[#1])-[#1])-[#6]([#8])-[#6](-[#1])-[#1])-[#6](-[#1])-[#1]  
mannich\_B(1)  
[#6]:1-2:[#6](:[#6]:[#6]:[#6](:[#6]:1-[#8]-[#6](-[#1])-[#1])-[#7](-[#6]:[#6]-[#8]-[#6](-[#1])-[#1])-[#6]-2(-[#1])-[#1])-[#1])-[#1]  
mannich\_catechol\_A(1)  
[#6]:1-2:[#6](:[#6](:[#6]:1-[#8]-[#6](-[#1])-[#1])-[#7](-[#6](-[#1])-[#1])-[#6]-2(-[#1])-[#1])-[#1])-[#8])-[#8]-[#1]  
melamine\_A(3)  
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melamine\_B(1)  
[#7]:1:[#6](:[#7]:[#6](:[#7]:[#6]:1-[#7](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#7](-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#7](-[#6]-[#1])-[#6]([#8])-[#6](-[#1])-[#1])-[#1])-[#1]  
misc\_aminal\_acid(1)  
[#6]:1:[#6]:[#6]-2:[#6](:[#6]:[#6]:1)-[#7](-[#6](-[#8]-[#6]-2)-[#6]([#8])-[#6](-[#8]-1),\$([#8]-[#1]))-[#6](-[#1])-[#1])-[#6]([#8])-[#6](-[#1])-[#1]  
misc\_aminoacid\_A(1)  
[#6;X4]-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#6]([#8])-[#7](-[#1])-[#6](-[#1])-[#6](-[#1])-[#1])-[#1])-[#6](-[#1])-[#16]-[#6](-[#1])-[#1])-[#1])-[#6]([#8])-[#6](-[#1])-[#1])-[#1])-[#1]  
misc\_anilide\_A(1)  
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misc\_anilide\_B(1)  
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misc\_anisole\_A(1)

[#6]:1(:[#6](:[#6]:2:[#6](:[#6](:[#6]:1-[#8]-[#6](-[#1]-[#1]-[#1]):[#6](:[#6](:[#6](:[#6]:2-[#7](-[#1])-  
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[#6](-[#1]-[#1]-[#1]-[#1]-[#1]-[#1]-[#8]-[#6](-[#1]-[#1])-[#1])  
misc\_anisole\_B(1)  
[#6]:1(:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1]-[#8]-[#6](-[#1]-[#1]-[#8]-[#6](-[#1]-[#1]-[#1]-[#1])-  
[#6](=[#8])-[#6](-[#1])-[#1]-[#7](-[#6](-[#1]-[#1]-[#6]:2:[#6]:[#6]:[#6](-[#6](-[#1]-[#1])[#6]:[#6]:2  
misc\_anisole\_C(1)  
[#7](-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1]-[#1]-[#8]-[#6](-[#1])-[#1]-[#1]-[#8]-[#6]-[#1])-  
[#1]-[#6](=[#8])-[#7](-[#1]-[#6](-[#1])-[#1]-[#6](-[#1])-[#1]-[#6](-[#1])-[#1]-[#7](-[#6](-[#1])-  
[#1]-[#1]-[#6]:[#6]  
misc\_cyclopropane(1)  
[#6]-1(-[#6](-[#1])-[#1]-[#6]-1(-[#1]-[#1])-[#6](=[#8])-[#7](-[#1]-[#6]:2:[#6]:[#6]:[#6](:[#6]:[#6]:2)-  
[#8]-[#6](-[#1])-[#1]-[#8]-[#16](=[#8])(=[#8])-[#6]:[#6]  
misc\_furan\_A(1)  
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[#8]-3)-[#1]-[#1])  
misc\_imidazole(1)  
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[#1]-[#6](-[#1])-[#1]-[#6]3n[#6]([#6](n3-[#6](-[#1])-[#1]-[#1]-[#1]-[#1])-[#1])  
misc\_naphthimidazole(1)  
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[#6]:3:[#6]:[#6](:[#6]:[#6]:3)-[#7](-[#1]-[#1]-[#7](-[#1]-[#1]):[#6]:[#6]:[#6]:[#6]:4  
misc\_phthal\_thio\_N(1)  
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misc\_pyridine\_OC(1)  
[#8]=[#6](-[#6]:1:[#6](:[#7]:[#6](:[#6]:1-[#1]-[#8]-[#6](-[#1])-[#1]-[#1]-[#8]-[#6](-[#1])-[#1]-  
[#1]-[#1]-[#7](-[#1]-[#6](-[#1])-[#6](-[#1]-[#1]-[#6](-[#1])-[#1])  
misc\_pyrrrole\_benz(1)  
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[#6](-[#1]-[#1]-[#1]-[#1]-[#6](-[#1])-[#1]-[#8]-[#6]:[#6])[#6]([#6](-[#1])[#6]([#6]2-[#1]-[#1]-[#1])  
misc\_pyrrrole\_thiaz(1)  
[#6]:1(:[#7]:[#6](:[#6](-[#1]):s:1)-[#6]:2:[#6]:[#6]:[#6]:[#6]:[#6]:2)-[#6](-[#1])-[#6](-[#1]-[#1]-[#6](-  
[#1])-[#1]-[#6](-[#1])-[#1]-[#7]-[#6](-[#1])-[#1]-[#6]:3:[#6]:[#6]:[#6]:[#7]:3-[#1])  
misc\_stilbene(1)  
[#6]-1(=[#6](-[#6](-[#6](-[#6](-[#6]-1(-[#1]-[#1])-[#1]-[#1]-[#6](=[#8])-[#6](-[#1]-[#6](=[#8])-  
[\$([#8-1]),\$([#8]-[#1])-[#1]-[#1]-[#6]:[#6]-[#6]:[#6]  
misc\_trityl\_A(1)  
[#6](-[#6]:[#6](-[#6]:[#6](-[#6]:[#6]-[#16]-[#6]:[#6]-[#6](=[#8])-[\$([#8-1]),\$([#8]-[#1])])  
misc\_urea\_A(1)  
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[#1]-[#6](-[#1])-[#1]-[#6](-[#1]-[#6](-[#1]-[#1]-[#6]:[#6]  
naphth\_ amino\_C(2)  
[#6]:2:[#6]:1:[#6]:[#6]:[#6]-3:[#6]:1:[#6](:[#6]:[#6]:2)-[#7](-[#7]=[#6]-3)-[#1])  
naphth\_ amino\_C\_bis(2)  
n1cc2cccc3cccc(n1[H])[#6]23  
naphth\_ amino\_D(2)  
[#6]:2:[#6]:1:[#6]:[#6]:[#6]-3:[#6]:1:[#6](:[#6]:[#6]:2)-[#7]-[#7]=[#7]-3  
naphth\_ ene\_ one\_A(1)  
[#6]:1:[#6]:[#6]:3:[#6]:2:[#6](:[#6]:1)-[#6](-[#6]=[#6](-[#6]:2:[#6]:[#6]:[#6]:3)-[#8]-[#6](-[#1]-[#1])=[#8]  
naphth\_ ene\_ one\_B(1)  
[#6]:1-3:[#6]:2:[#6](:[#6](:[#6]:[#6]:1)-[#7]:[#6]:[#6]:[#6]:2-[#6](-[#6]=[#6]-3-[#6](-[F])(-  
[F])=[#8]  
naphth\_ ene\_ one\_C(1)  
[#6]:2(:[#6]:1:[#6]:[#6]:[#6]-3:[#6]:1:[#6](:[#6]:[#6]:2)-[#6]=[#6]-[#6]-3=[#7]-[#7]  
phenol\_sulfite\_A(1)  
[#6](-[#6]:1:[#6]:[#6]:[#6](:[#6]:[#6]:1)-[#8]-[#1])(-[#6]:2:[#6]:[#6]:[#6](:[#6]:[#6]:2)-[#8]-[#1]-[#8]-  
[#16](=[#8])=[#8]  
phthalimide\_misc(2)  
[#7]-2(-[#6]([#8])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1]-[#6](=[#8])-[\$([#8-1]),\$([#8]-[#1])]-[#1])-  
[#1]-[#6]-2=[#8])-[#6]:3:[#6](:[#6]:[#6](:[#6](:[#6]:3)-[#1]-[#8])-[#1])  
pyrazole\_ amino\_A(1)  
[#6]1[#6](-[#7](-[#1]-[#1])[#7][#7][#6]1-[#6]2[#6](-[#6](-[#1]-[#1])o[#6]([#6]2-[#1]-[#1])  
pyrazole\_ amino\_B(1)  
s1[#6][#6][#7][#6]1-[#6]2[#6]([#7]([#7][#6]2-[#1]-[#1]-[#7](-[#1]-[#1])  
pyrrrole\_C(8)  
[#7]1(-[#6;X4])[#6]([#6](-[#1])[#6]([#6]1-[#6](-[#1])-[#1]-[#7](-[#1]-[#6](=[#16])-[#7]-[#1]-[#1]-[#1])  
pyrrrole\_D(5)  
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pyrrrole\_E(5)  
[#7]2(-[#6]:1:![#1]:![#6&!#1]:![#1]:[#6]:1-[#1])[#6]([#6](-[#1])[#6]([#6]2-[#6;X4]-[#1]-[#6;X4])  
pyrrrole\_F(5)  
[#7]2(-[#6]:1:[#6](-[#6]#[#7]):[#6]:[#6]:![#6&!#1]:1)[#6]([#6](-[#1])[#6]([#6]2-[#1]-[#1])  
pyrrrole\_G(4)  
[#7]2(-[#6]:1:[#6](:[#6]:[#6](:[#6](:[#6]:1)-[#1]-[\$([#7](-[#1]-[#1]),\$([#6]:[#7]))-[#1])[#6]([#6](-  
[#1])[#6]([#6]2-[#1]-[#1]-[#1])

```

pyrrole_H(3)
[#7]1-2[#6][#6][#6][#6]1-[#6]=[#7](-[#6])-[#6]-[#6]-2
pyrrole_I(2)
[#7]2(-[#6](-[#1])-[#1])[#6]-1[#6](-[#6]:[#6]-[#6]-1=[#8])[#6][#6]2-[#6](-[#1])-[#1]
pyrrole_J(1)
[#6]1([#6]-2[#6]([#6]([#7]1-[#6](-[#8])=[#8])-[#6](-[#1])-[#1])-[#16]-[#6](-[#1])-[#1])-[#16]-2)-[#6](-
[#1])-[#1]
pyrrole_K(1)
[#6]1([#6]([#6]([#6]([#7]1-[#1])-[#6]:2:[#6](:[#6](:[#6](:[#6](:[#6]:2-[#1])-[#1])-[#1])-[#1])-[#1])-[#6](-
[#1])-[#1])-[#1])-[#6](=[#8])-[#6](-[#8]-1),[#6](-[#1]))]
pyrrole_L(1)
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[#1])-[#6](-[#1])-[#1])-[#6](=[#8])-[#8]-[#6](-[#1])-[#1]
pyrrole_M(1)
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pyrrole_N(1)
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[#6]-[#1])-[#1])-[#6]-[#1]
pyrrole_O(1)
[#7]1(-[#6](-[#1])-[#1])[#6]([#6](-[#6](=[#8])-[#6])[#6]([#6]1-[#6]:[#6]-[#6]-[#6](-[#1])-[#1])
quinone_B(5)
[#6]:1:[#6]:[#6]-2:[#6](:[#6]:[#6]:1)-[#6](-[#6]3[#6][#6][#6][#6]4[#7]o[#6]-2[#6]34)=[#8]
quinone_C(2)
[#8]=[#6]-3-[#6]:1:[#6](:[#6]:[#6]:[#6]:[#6]:1)-[#6]-2=[#6](-[#8]-[#1])-[#6]([#6](-[#7])-[#6]:4:[#6]-2:[#6]-
3:[#6]:[#6]:[#6]:4
quinone_D(2)
[#6]-1(-[#6]=,:[#6]-[#6]=,:[#6]-[#6]-1=[!#6&!#1])=[!#6&!#1]
rhod_sat_B(3)
[#7]-2(-[#6]:1:[#6]:[#6]:[#6]:[#6]:1-[#6](-[#1])-[#1])-[#6]([#6]1-[#6]:[#6]-[#6]-[#6](-[#1])-[#1])-[
!#1]:[!#1]:[!#1]:[!#1]:[!#1])-[#6](-[#1])-[#6]-2=[#8]
rhod_sat_C(3)
[#7]-2(-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#6]([#6](-[#7])-[#6]=[#8])-[#16]-[#6](-[#1])-[#1])-[#6]-2=[#8]
rhod_sat_D(3)
[#7]-2(-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#6]([#6](-[#8])-[#16]-[#6](-[#1])-[#6](-[#1])-[#1])-[#6]([#6]1-
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rhod_sat_E(1)
[#7]-4(-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#6]([#6](-[#8])-[#16]-[#6](-[#1])-[#7](-[#1])-
[#6]:2:[#6]:[#6]:[#6]:3:[#6]:[#6]:[#6]:[#6]:2:3)-[#6]-4=[#8]
rhod_sat_F(1)
[#7]-2(-[#6]:1:[#6]:[#6]:[#6]:[#6]:1)-[#6]([#6](-[#8])-[#16]-[#6](-[#1])-[#1])-[#6]-2=[#16]
rhod_sat_imine_A(1)
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[#6](-[#1])-[#1])-[#6]-3=[#8]
steroid_A(2)
[#8]=[#6]-4-[#6]-[#6]-[#6]-3-[#6]-2-[#6]([#6](-[#8])-[#6]-[#6]-1-[#6]-[#6]-[#6]-1-[#6]-2-[#6]-[#6]-[#6]-
3=[#6]-4
styrene_A(13)
[#6]-2-[#6]-[#6]:1:[#6](:[#6]:[#6]:[#6]:[#6]:1)-[#6](-[#6]:3:[#6]:[#6]:[#6]:[#6]:[#6]:2:3)=[#6]-[#6]
styrene_B(8)
[#6]:1:[#6]:[#6]-2:[#6](:[#6]:[#6]:1)-[#6](-[#6]:3:[#6](-[#6]:3:[#6](-[#6]:2:3)-[#6]-[#6]:2:3)-
[!#6&!#1]:[!#1]:[!#1]:[!#1]:[!#1])-[#6]-[#6]
styrene_C(4)
[#6]:1:[#6]:[#6]-2:[#6](:[#6]:[#6]:1)-[#6]-[#16]-[#6]3[#6](-[#6]-2=[#6])[#6][#6]s3
styrene_anil_A(1)
[#6]:1:[#6]:[#6]-3:[#6](:[#6]:[#6]:1)-[#6]:2:[#6]:[#6]:[#6](:[#6]:[#6]:2-[#6]-3=[#6](-[#1])-[#6]-[#7](-
[#1])-[#1]
styrene_imidazole_A(1)
[#6]([#6](-[#1])-[#6](-[#1])-[#1])-[#7]:1:[#6](:[#7]:[#6](:[#6]:1-[#1])-[#1])-[#1])-[#6]:[#6]-[#6]:[#6]
sulfonamide_C(5)
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[!#6&!#1])-[#1])-[#8]-[#6](-[#8]-3)-[#1])-[#1])-[#1])-[#1]
sulfonamide_D(2)
[#6]:1:[#6]:[#6](:[#6]:[#6]:1-[#7](-[#1])-[#16]([#6](-[#8])=[#8])-[#7](-[#1])-[#16]([#6](-[#8])=[#8])=[#8]
sulfonamide_E(2)
[#6]:[#6]-[#7](-[#1])-[#16]([#6](-[#8])=[#8])-[#7](-[#1])-[#6]:[#6]
sulfonamide_F(1)
[#8]=[#16]([#6](-[#8])-[#7](-[#1])-[#6]1[#7][#6]([#6]s1)-[#6]:[#6]
sulfonamide_G(1)
[#6](-[#1])-[#1])-[#1])-[#6]:1:[#6](:[#6](:[#6](:[#6](:[#7]:1)-[#7](-[#1])-[#16](-
[#6]:2:[#6](:[#6](:[#6](:[#6]:2-[#1])-[#1])-[#1])-[#8]-[#6](-[#1])-[#1])-[#6](-[#1])-[#1])-[#6](-[#1])-[
[#1])-[#1])-[#1])-[#8])-[#8]-[#1])-[#1])-[#1]
sulfonamide_H(1)
[#6]:1:[#6](:[#6](:[#6](:[#6](:[#6]:1-[#1])-[#1])-[#7](-[#1])-[#1])-[#1])-[#1])-[#16]([#6](-[#8])=[#8])-[#7](-
[#1])-[#6]:2:[#6]:[#7]:[#6](:[#6](:[#6]:2-[#1])-[#1])-[#1])-[#1]
sulfonamide_I(1)
[#6]([#6](-[#8])=[#8])-[#6]:1:[#6]:[#7](-[#6](-[#1])-[#1])-[#6]:[#7]:1)-[#7](-[#1])-[#6]:2:[#6]:[#7]
sulfonamide_J(1)

```

[#7]3(-[#6]:1:[#6]:[#6]:[#6]:[#6]:[#6]:1-[#7](-[#1])-[#16](=[#8])(=[#8])-  
[#6]:2:[#6]:[#6]:[#6]:s:2)[#6]([#6](-[#1])[#6]([#6]3-[#1])-[#1])-[#1])  
tert\_butyl\_A(2)  
[#6](-[#1])(-[#1])(-[#1])-[#6](-[#6](-[#1])(-[#1])-[#1])(-[#6](-[#1])(-[#1])-[#1])-  
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[#1])(-[#1])-[#1])-[#8]-[#6](-[#1])-[#7])-[#1])  
tert\_butyl\_B(1)  
[#6](-[#1])(-[#1])(-[#1])-[#6](-[#6](-[#1])(-[#1])-[#1])(-[#6](-[#1])(-[#1])-[#1])-  
[#6]:1:[#6]([#6]:[#6]:[#6]([#6]:[#6]:1-[#8]-[#1])-[#6](-[#6](-[#1])(-[#1])-[#1])(-[#6](-[#1])(-[#1])-[#1])-  
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[#1])  
tetrazole\_A(1)  
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thiazole\_amine\_G(2)  
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thiazole\_amine\_N(1)  
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thio\_aldehyd\_A(3)  
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thio\_amide\_A(6)  
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thio\_amide\_B(2)  
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thio\_amide\_D(2)  
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thio\_amide\_E(1)  
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thio\_amide\_F(1)  
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thio\_carbam\_A(1)

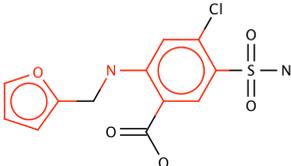
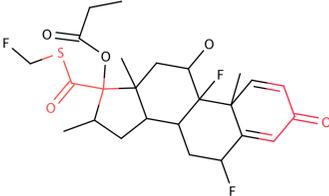
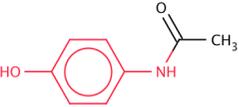
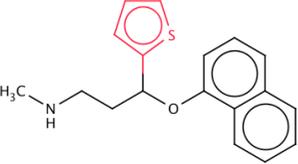
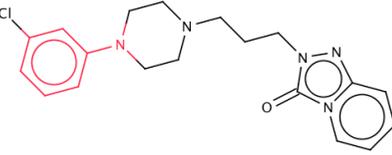
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thio\_cyano\_A(1)  
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thio\_ene\_amine\_A(1)  
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thio\_est\_cyano\_A(1)  
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thio\_ester\_A(5)  
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thio\_ester\_B(4)  
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thio\_ester\_C(2)  
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thio\_imide\_A(1)  
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thio\_imine\_ium(2)  
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thio\_keto\_het(2)  
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thio\_thiomorph\_Z(1)  
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thio\_urea\_A(12)  
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thio\_urea\_B(9)  
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thio\_urea\_C(9)  
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thio\_urea\_D(8)  
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thio\_urea\_E(7)  
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thio\_urea\_F(6)  
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thio\_urea\_G(5)  
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thio\_urea\_H(3)  
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thio\_urea\_I(3)  
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thio\_urea\_J(2)  
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thio\_urea\_K(2)  
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thio\_urea\_L(1)  
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thio\_urea\_M(1)  
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thio\_urea\_O(1)  
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thio\_urea\_P(1)  
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thio\_urea\_Q(1)  
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thio\_urea\_R(1)  
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thiophene\_C(3)

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thiophene\_E(2)  
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thiophene\_F(1)  
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thiophene\_amino\_B(12)  
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thiophene\_amino\_B\_bis(12)  
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thiophene\_amino\_C(7)  
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thiophene\_amino\_D(3)  
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thiophene\_amino\_E(2)  
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thiophene\_amino\_F(2)  
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thiophene\_amino\_G(2)  
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thiophene\_amino\_H(2)  
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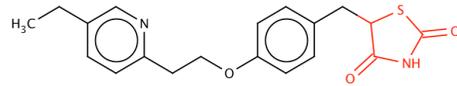
Supplementary.Table.S2

FAF-Drugs3 Pre-Defined Filters								
Descriptors	R03	R05	Drug-Like	Lead-Like	REOS	ZINC	CNS	Respiratory
<b>MW</b>	≤ 300	(≤ 500)	100 - 600	150 - 400	200 - 500	60 - 600	135 - 582	240 - 520
<b>logP</b>	-3 to 3	(≤ 5)	-3 to 6	-3 to 4	-5 to 5	-4 to 6	-0.2 to 6.1	-2 to 4.7
<b>HBA</b>	≤ 3	(≤ 10)	≤ 12	≤ 7	≤ 10	≤ 11	≤ 5	-
<b>HBD</b>	≤ 3	(≤ 5)	≤ 5	≤ 4	≤ 5	≤ 6	≤ 3	-
<b>HBonds</b>	-	-	-	-	-	-	-	6 - 12
<b>tPSA</b>	≤ 60	-	≤ 180	≤ 160	≤ 150	≤ 150	3 - 118	51 - 135
<b>Rotatable Bonds</b>	≤ 3	-	≤ 11	≤ 9	≤ 8	≤ 12	-	3 - 8
<b>Rigid Bonds</b>	-	-	≤ 30	≤ 30	-	≤ 50	-	-
<b>Rings</b>	-	-	≤ 6	≤ 4	-	≤ 7	-	1 - 5
<b>MaxSizeSystemRing</b>	-	-	≤ 18	≤ 18	-	≤ 12	-	-
<b>Carbons</b>	-	-	3 - 35	3 - 35	-	≥ 3	-	-
<b>HeteroAtoms</b>	-	-	01 - 15	01 - 15	-	≥ 0	-	-
<b>H/C Ratio</b>	-	-	0.1 to 1.1	0.1 to 1.1	-	≤ 2.0	-	-
<b>Charges</b>	-	-	≤ 3	≤ 3	-	≤ 3	-	-
<b>TotalCharge</b>	-	-	-2 to 2	-2 to 2	-2 to 2	-2 to 2	-	-
<b>R05 Violations</b>	-	2	-	-	-	-	-	-
<b>StereoCenters</b>	-	-	-	≤ 2	-	-	-	-

Supplementary.Table.S3

Drug	Depiction	FAF-Drugs3 Alert	Stepan <i>et al.</i>
Furosemide		Furan Masked Aniline	Furan Aniline
Fluticasone		Michael acceptor double Thioester	Michael Acceptor Thioester Alkylhalide Phenol
Acetaminophen		Masked Aniline para-aminophenol para-hydroxyanilines Phenol	P-Alkylaromatic Ether P-Hydroxy-acetAniline
Duloxetine		Thiophene	Thiophene
Trazodone		Aniline	Aniline

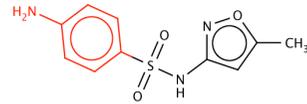
Pioglitazone



Thiazolidinedione  
Thioester

Thiazolidinedione

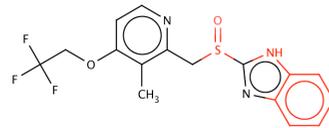
Sulfamethoxazole



Aniline

Aniline  
P-Alkylaniline  
Dialkoxyaromatic

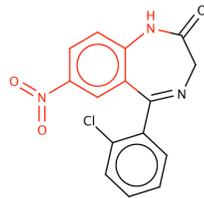
Lansoprazole



Aniline  
Sulfoxide

Aniline  
O-Alkylaromatic ether

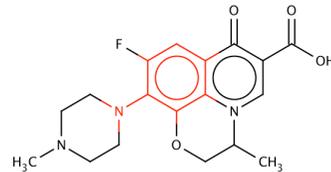
Clonazepam



Aniline  
Nitro  
Nitrobenzene

P-Nitroaniline

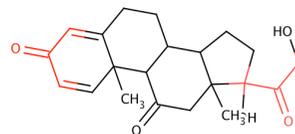
Levofloxacin



Aniline

O-Alkoxyaniline

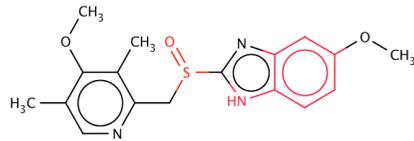
Prednisone



Michael acceptors double  
n-acylated azoles

Michael acceptor

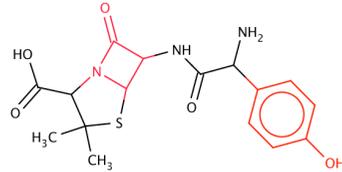
Omeprazole



Aniline  
Sulfoxide

Aniline  
p-Alkylaromatic ether

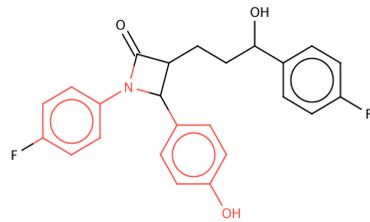
Amoxicillin



Betalactams  
Phenol

$\beta$ -lactam  
Phenol

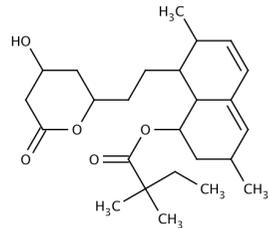
Ezetimibe



Masked Aniline  
Phenol

Aniline  
Olefin  
Phenol

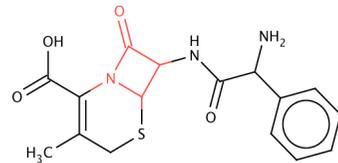
Simvastatin



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Aniline  
Phenol  
Olefin

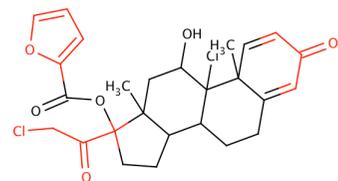
Cephalexin



Betalactams

$\beta$ -lactam

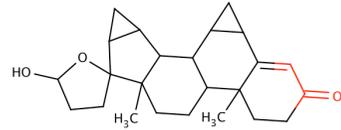
Mometasone Furoate



Alkyl halide nof  
Michael\_acceptors\_double  
Alphahalo-ketone carbonyl  
Furan  
n-acylated azoles

Furan  
Michael acceptor  
Alkylhalide

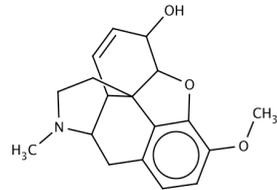
Drospirenone



Michael acceptors double

Michael acceptor  
Alkyne  
Phenol

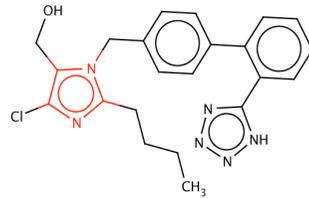
Codeine



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P-Alkylaromatic éther  
P-Hydroxy-acetanilide

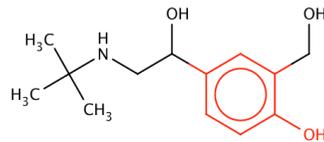
Losartan



Imidazole

Alkylimidazole

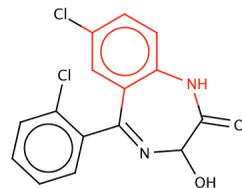
Albuterol



Phenol

Phenol

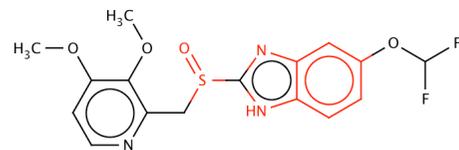
Lorazepam



Masked Aniline

Aniline

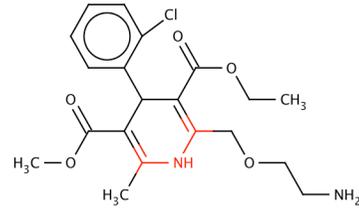
Pantoprazole



Aniline  
Sulfoxide

Aniline  
Dialkoxyaromatic

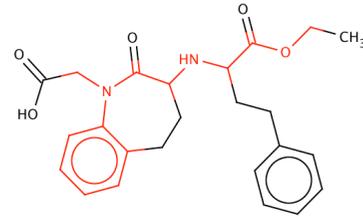
Amlodipine



Michael acceptors double

Aniline

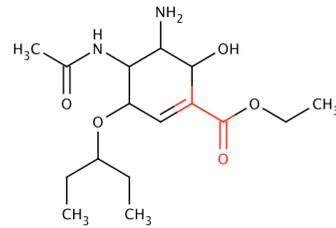
Benazepril



Crown 2-2  
Masked Aniline

Aniline

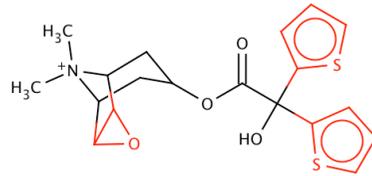
Seltamivir



Michael acceptors double

Michael Acceptor

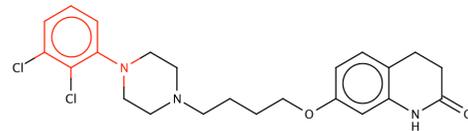
Tiotropium



Epoxide  
Thiophene

Bromide  
Thiophene  
Epoxide

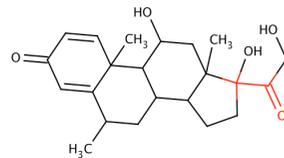
Aripiprazole



Aniline

Aniline  
Aniline

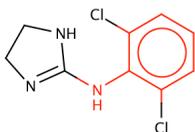
Methylprednisolone



Michael acceptors double  
n-acylated azoles

Michael acceptor

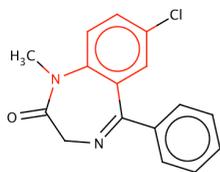
Clonidine



Masked Aniline

Aniline

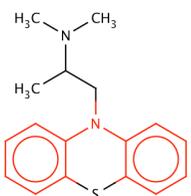
Diazepam



Masked Aniline

Aniline

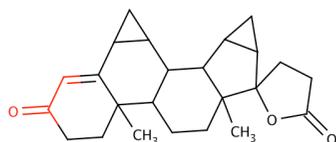
Promethazine



Masked Aniline

Aniline

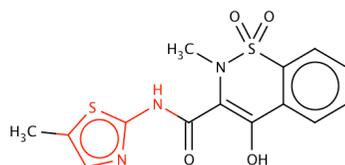
Drospirenone



Michael acceptors double

Michael acceptor

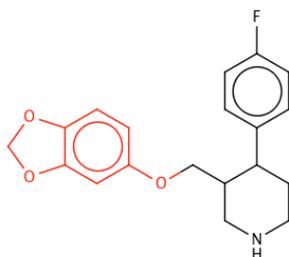
Meloxicam



1,2-aminothiazole  
Thiazole

2-Aminothiazole

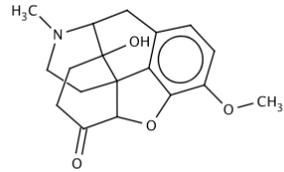
Paroxetine



Benzodioxolane  
Michael acceptors double

1 3-Benzodioxole

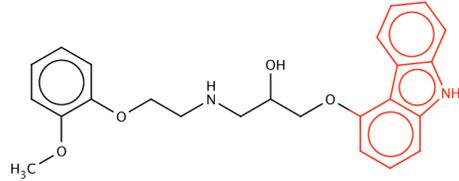
Oxycontin



/

P-Alkylaromatic ether

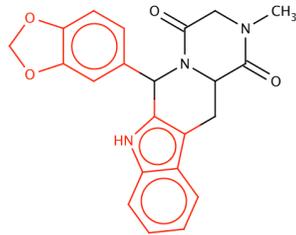
Carvedilol



Aniline  
Pyrrole

Aniline  
Dialkoxyaromatic

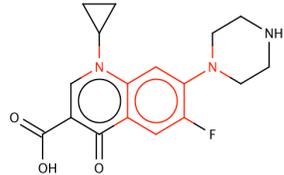
Tadalafil



Benzodioxolane  
Aniline  
Pyrrole

Aniline  
1,3-Benzodioxole

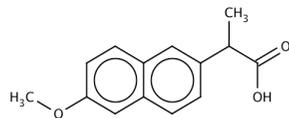
Ciprofloxacin



Aniline

Aniline

Naproxen



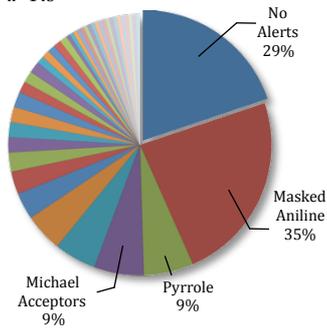
/

Arylacetic acid

## Supplementary.Figure.S4

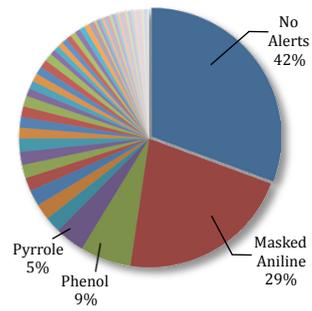
### Cardiology

n= 143



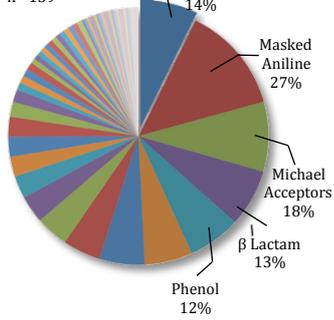
### Neurology

n= 221



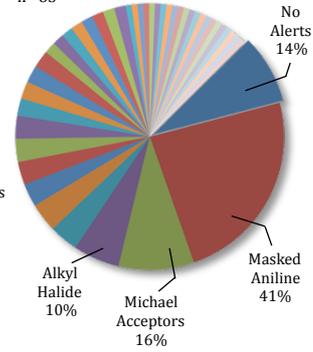
### Infectious

n= 159



### Oncology

n= 83



Supplementary.Figure.S5

